



FIGURE 1

Amino acid sequence for full-length E. coli IspA (residues 16-314) with an N-terminal His-tag (residues 1-15, underlined)

[SEQ. ID No. 1]

MGSDKI IHHHHHHTLMDFPQQLEACVKQANQALSRFIAPLPFQNTPVVETMQYGALLGGK
RLRPFLVYATGHMFGVSTNTLDAPAAAVECIHAYSLIHDDLPAMDDDDLRRLPTCHVKF
GEANAILAGDALQTLAFSILSDADMPEVSDRDRISMISELASASGIAGMCGGQALLDAAE
GKHVPLDALERIHRHKTGALIRAAVRLGALSAGDKRRRALPVLDKYAESIGLAFQVQDDI
LDVVGDTATLGKRQGADQQLGKSTYPALLGLEQARKKARDLIIDARQSLKQLAEQSLDTS
ALEALADYIIQRNK

cDNA sequence encoding IspA (residues 46-945) with an N-terminal His-tag (residues 1-45; underlined)

[SEQ. ID No. 2]

ATGGGATCTGATAAAATTATTCACCACCATCACCACCATACCC~~TT~~TATGGACTTCCGCAG
CAACTCGAACGCTCGTTAACGAGGCCAACCAAGGCCGCTGAGCCGTTTATGCC~~CCC~~CACTG
CCCTTCAGAACACTCCCGTGGTCGAAACCATGCAGTATGCCGCAATTATTAGGTGGTAAG
CGCCTGCGACCTTCTGGTTATGCCACCGTCATATGTTCCGGCTTAGCACAAACACG
CTGGACGCACCCGCTGCCGCCGTTGAGTGATCCACGCTTACTCATTAATTGATGATGAT
TTACCGGAATGGATGATGACGATCTCGCTCGCGGTTGCCAACCTGCCATGTGAAGTTT
GGCGAACGAAACCGGATTCTCGCTGGCGACGCTTACAAACGCTGGCTTCGATTTA
AGCGATGCCGATATGCCGGAAAGTGTGGACCGCGACAGAATTGATGATTTCTGAACTG
GCGAGCGCCAGTGGTATTGCCGGATGTGGCTGGCAGGCATTAGATTAGACGCGGAA
GGCAAACACGTACCTCTGGACGCCCTTGAGCGTATTGATCGTCATAAAACCGGCCATTG
ATTGCGCCGCCGTTGCCCTGGTGCATTAAGCGCCGGAGATAAAGGACGTCGTGCTCTG
CCGGTACTCGACAAGTATGCGAGAGACATCGGCCCTGCCCTCCAGGTTAGGATGACATC
CTGGATGTGGTGGGAGATACTGCAACGTTGGAAAACGCCAGGGTGCCGACCAGCAACTT
GGTAAAAGTACCTACCCCTGCACTCTGGTCTTGAGCAAGCCGGAAAGAAAGCCGGGAT
CTGATCGACGATGCCGTCACTCGCTGAAACAATGGCTGAACAGTCACTCGATACTCG
GCACTGGAAGCGCTAGCGGACTACATCATCCAGCGTAATAAATAA

FIGURE 3

LEGEND

Column headings from left to right are (A)‘Atom Number’, (B)‘Atom Type’, (C)‘Amino Acid’, (D)‘Chain Identifier’, (E)‘Amino Acid Number’, (F)‘X Coordinate’, (G)‘Y Coordinate’, (H)‘Z Coordinate’, (I)‘Occupancy’ (OCC) and (J)‘B factor’.

A	B	C	D	E	F	G	H	I	J
1	N	MET	A	16	65.564	50.628	-5.933	1.00	45.23
3	CA	MET	A	16	65.166	51.178	-7.255	1.00	44.87
5	CB	MET	A	16	64.933	50.049	-8.267	1.00	45.30
8	CG	MET	A	16	65.153	50.446	-9.726	1.00	47.01
11	SD	MET	A	16	66.181	49.252	-10.631	1.00	50.95
12	CE	MET	A	16	64.933	48.059	-11.220	1.00	50.52
16	C	MET	A	16	63.907	52.030	-7.120	1.00	43.94
17	O	MET	A	16	63.880	53.159	-7.610	1.00	44.23
20	N	ASP	A	17	62.875	51.491	-6.466	1.00	42.41
22	CA	ASP	A	17	61.591	52.188	-6.366	1.00	41.35
24	CB	ASP	A	17	60.409	51.226	-6.459	1.00	41.74
27	CG	ASP	A	17	59.134	51.926	-6.899	1.00	43.33
28	OD1	ASP	A	17	58.448	52.535	-6.037	1.00	46.33
29	OD2	ASP	A	17	58.753	51.939	-8.093	1.00	45.52
30	C	ASP	A	17	61.486	52.990	-5.079	1.00	39.80
31	O	ASP	A	17	61.195	52.441	-4.005	1.00	38.54
32	N	PHE	A	18	61.672	54.298	-5.210	1.00	38.05
34	CA	PHE	A	18	61.858	55.146	-4.050	1.00	36.90
36	CB	PHE	A	18	62.429	56.514	-4.427	1.00	36.92
39	CG	PHE	A	18	63.016	57.233	-3.260	1.00	36.41
40	CD1	PHE	A	18	64.116	56.707	-2.609	1.00	37.05
42	CE1	PHE	A	18	64.658	57.340	-1.502	1.00	36.55
44	CZ	PHE	A	18	64.098	58.493	-1.036	1.00	36.07
46	CE2	PHE	A	18	62.988	59.025	-1.664	1.00	36.56
48	CD2	PHE	A	18	62.442	58.392	-2.768	1.00	36.65
50	C	PHE	A	18	60.632	55.314	-3.158	1.00	35.80
51	O	PHE	A	18	60.769	55.198	-1.949	1.00	35.17
52	N	PRO	A	19	59.456	55.618	-3.712	1.00	34.90
53	CA	PRO	A	19	58.239	55.676	-2.889	1.00	34.06
55	CB	PRO	A	19	57.123	55.861	-3.924	1.00	34.29
58	CG	PRO	A	19	57.782	56.558	-5.047	1.00	34.27
61	CD	PRO	A	19	59.176	55.993	-5.114	1.00	34.77
64	C	PRO	A	19	58.008	54.418	-2.039	1.00	33.38
65	O	PRO	A	19	57.585	54.564	-0.895	1.00	32.65
66	N	GLN	A	20	58.279	53.228	-2.579	1.00	32.48
68	CA	GLN	A	20	58.126	51.981	-1.815	1.00	32.23
70	CB	GLN	A	20	58.188	50.746	-2.732	1.00	32.68
73	CG	GLN	A	20	56.883	50.493	-3.534	1.00	35.01
76	CD	GLN	A	20	56.611	49.011	-3.811	1.00	39.06
77	OE1	GLN	A	20	55.463	48.546	-3.685	1.00	41.57
78	NE2	GLN	A	20	57.654	48.270	-4.193	1.00	39.95
81	C	GLN	A	20	59.177	51.869	-0.700	1.00	30.90
82	O	GLN	A	20	58.892	51.363	0.379	1.00	30.03

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
83	N	GLN	A	21	60.385	52.351	-0.959	1.00	29.82
85	CA	GLN	A	21	61.426	52.370	0.058	1.00	29.68
87	CB	GLN	A	21	62.783	52.738	-0.560	1.00	29.82
90	CG	GLN	A	21	63.366	51.647	-1.494	1.00	31.98
93	CD	GLN	A	21	63.920	50.425	-0.746	1.00	34.89
94	OE1	GLN	A	21	64.483	49.512	-1.360	1.00	36.76
95	NE2	GLN	A	21	63.762	50.412	0.572	1.00	37.29
98	C	GLN	A	21	61.065	53.323	1.204	1.00	28.61
99	O	GLN	A	21	61.214	52.973	2.372	1.00	28.03
100	N	LEU	A	22	60.588	54.513	0.863	1.00	27.80
102	CA	LEU	A	22	60.120	55.472	1.848	1.00	27.76
104	CB	LEU	A	22	59.582	56.740	1.169	1.00	28.15
107	CG	LEU	A	22	60.595	57.714	0.543	1.00	29.56
109	CD1	LEU	A	22	59.880	58.764	-0.297	1.00	30.48
113	CD2	LEU	A	22	61.447	58.392	1.611	1.00	30.42
117	C	LEU	A	22	59.036	54.861	2.736	1.00	27.31
118	O	LEU	A	22	59.099	54.975	3.950	1.00	26.43
119	N	GLU	A	23	58.057	54.185	2.145	1.00	27.14
121	CA	GLU	A	23	56.973	53.627	2.952	1.00	27.44
123	CB	GLU	A	23	55.760	53.232	2.101	1.00	28.34
126	CG	GLU	A	23	54.798	52.234	2.759	1.00	31.44
129	CD	GLU	A	23	53.961	52.789	3.912	1.00	35.82
130	OE1	GLU	A	23	52.791	52.370	4.024	1.00	38.87
131	OE2	GLU	A	23	54.448	53.597	4.738	1.00	38.87
132	C	GLU	A	23	57.465	52.462	3.805	1.00	26.15
133	O	GLU	A	23	57.040	52.322	4.949	1.00	25.29
134	N	ALA	A	24	58.357	51.642	3.254	1.00	25.31
136	CA	ALA	A	24	59.018	50.578	4.013	1.00	24.72
138	CB	ALA	A	24	60.019	49.847	3.153	1.00	25.46
142	C	ALA	A	24	59.728	51.160	5.230	1.00	24.33
143	O	ALA	A	24	59.610	50.636	6.331	1.00	23.33
144	N	CYS	A	25	60.438	52.263	5.025	1.00	23.38
146	CA	CYS	A	25	61.130	52.944	6.115	1.00	23.00
148	CB	CYS	A	25	62.029	54.056	5.578	1.00	23.11
151	SG	CYS	A	25	62.861	54.980	6.885	1.00	21.11
152	C	CYS	A	25	60.147	53.499	7.162	1.00	22.39
153	O	CYS	A	25	60.368	53.344	8.351	1.00	22.44
154	N	VAL	A	26	59.051	54.105	6.725	1.00	22.24
156	CA	VAL	A	26	58.056	54.638	7.651	1.00	22.18
158	CB	VAL	A	26	56.889	55.349	6.902	1.00	22.57
160	CG1	VAL	A	26	55.697	55.610	7.815	1.00	22.85
164	CG2	VAL	A	26	57.368	56.650	6.293	1.00	22.19
168	C	VAL	A	26	57.534	53.530	8.580	1.00	21.91
169	O	VAL	A	26	57.440	53.722	9.789	1.00	21.65
170	N	LYS	A	27	57.235	52.369	8.011	1.00	21.41
172	CA	LYS	A	27	56.741	51.236	8.779	1.00	21.24
174	CB	LYS	A	27	56.273	50.127	7.836	1.00	22.15
177	CG	LYS	A	27	54.982	50.454	7.081	1.00	24.03
180	CD	LYS	A	27	54.467	49.210	6.340	1.00	28.62
183	CE	LYS	A	27	53.133	49.458	5.596	1.00	31.91
186	NZ	LYS	A	27	53.166	48.924	4.184	1.00	33.67
190	C	LYS	A	27	57.798	50.693	9.737	1.00	20.33

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
191	O	LYS	A	27	57.499	50.428	10.910	1.00	19.84
192	N	GLN	A	28	59.022	50.536	9.244	1.00	19.37
194	CA	GLN	A	28	60.116	50.039	10.073	1.00	19.22
196	CB	GLN	A	28	61.413	49.892	9.264	1.00	19.05
199	CG	GLN	A	28	62.596	49.326	10.078	1.00	19.21
202	CD	GLN	A	28	62.485	47.814	10.392	1.00	20.65
203	OE1	GLN	A	28	63.076	47.320	11.375	1.00	22.34
204	NE2	GLN	A	28	61.792	47.087	9.537	1.00	16.09
207	C	GLN	A	28	60.340	50.985	11.258	1.00	18.67
208	O	GLN	A	28	60.392	50.549	12.386	1.00	18.19
209	N	ALA	A	29	60.465	52.278	10.985	1.00	18.55
211	CA	ALA	A	29	60.748	53.271	12.026	1.00	18.70
213	CB	ALA	A	29	61.022	54.625	11.403	1.00	18.98
217	C	ALA	A	29	59.626	53.382	13.036	1.00	19.64
218	O	ALA	A	29	59.875	53.535	14.238	1.00	19.64
219	N	ASN	A	30	58.386	53.300	12.564	1.00	19.52
221	CA	ASN	A	30	57.232	53.369	13.464	1.00	19.96
223	CB	ASN	A	30	55.920	53.446	12.688	1.00	19.83
226	CG	ASN	A	30	55.652	54.816	12.118	1.00	22.13
227	OD1	ASN	A	30	56.322	55.792	12.458	1.00	23.82
228	ND2	ASN	A	30	54.638	54.904	11.249	1.00	23.36
231	C	ASN	A	30	57.177	52.190	14.405	1.00	19.86
232	O	ASN	A	30	56.847	52.343	15.573	1.00	19.83
233	N	GLN	A	31	57.474	51.010	13.878	1.00	20.51
235	CA	GLN	A	31	57.584	49.779	14.679	1.00	21.34
237	CB	GLN	A	31	57.921	48.608	13.760	1.00	21.77
240	CG	GLN	A	31	57.882	47.246	14.412	1.00	24.92
243	CD	GLN	A	31	58.025	46.137	13.385	1.00	29.08
244	OE1	GLN	A	31	59.120	45.918	12.832	1.00	33.06
245	NE2	GLN	A	31	56.929	45.446	13.112	1.00	31.52
248	C	GLN	A	31	58.683	49.902	15.737	1.00	21.05
249	O	GLN	A	31	58.488	49.550	16.899	1.00	20.55
250	N	ALA	A	32	59.839	50.384	15.310	1.00	20.90
252	CA	ALA	A	32	60.957	50.629	16.213	1.00	21.59
254	CB	ALA	A	32	62.129	51.176	15.451	1.00	21.36
258	C	ALA	A	32	60.539	51.598	17.315	1.00	21.65
259	O	ALA	A	32	60.696	51.304	18.475	1.00	22.05
260	N	LEU	A	33	59.999	52.750	16.940	1.00	22.61
262	CA	LEU	A	33	59.575	53.760	17.906	1.00	23.19
264	CB	LEU	A	33	58.931	54.937	17.175	1.00	23.47
267	CG	LEU	A	33	59.879	55.966	16.574	1.00	24.21
269	CD1	LEU	A	33	59.165	56.759	15.502	1.00	24.68
273	CD2	LEU	A	33	60.391	56.887	17.685	1.00	26.09
277	C	LEU	A	33	58.555	53.183	18.890	1.00	24.35
278	O	LEU	A	33	58.659	53.391	20.094	1.00	23.66
279	N	SER	A	34	57.567	52.471	18.356	1.00	25.27
281	CA	SER	A	34	56.513	51.879	19.172	1.00	26.76
283	CB	SER	A	34	55.480	51.162	18.295	1.00	27.01
286	OG	SER	A	34	54.789	52.077	17.470	1.00	28.06
288	C	SER	A	34	57.070	50.896	20.194	1.00	27.73
289	O	SER	A	34	56.597	50.849	21.316	1.00	28.77
290	N	ARG	A	35	58.071	50.117	19.802	1.00	28.38

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
292	CA	ARG	A	35	58.649	49.117	20.688	1.00	29.15
294	CB	ARG	A	35	59.580	48.182	19.915	1.00	29.68
297	CG	ARG	A	35	58.842	47.176	19.053	1.00	33.37
300	CD	ARG	A	35	59.681	46.648	17.895	1.00	36.27
303	NE	ARG	A	35	59.113	45.445	17.291	1.00	39.06
305	CZ	ARG	A	35	59.778	44.630	16.473	1.00	41.04
306	NH1	ARG	A	35	61.046	44.878	16.153	1.00	42.52
309	NH2	ARG	A	35	59.174	43.564	15.970	1.00	42.39
312	C	ARG	A	35	59.426	49.761	21.828	1.00	28.40
313	O	ARG	A	35	59.480	49.210	22.926	1.00	27.74
314	N	PHE	A	36	60.045	50.910	21.557	1.00	27.61
316	CA	PHE	A	36	60.785	51.634	22.587	1.00	27.39
318	CB	PHE	A	36	61.853	52.533	21.960	1.00	27.18
321	CG	PHE	A	36	62.924	51.766	21.240	1.00	25.69
322	CD1	PHE	A	36	63.214	52.029	19.918	1.00	25.01
324	CE1	PHE	A	36	64.194	51.311	19.253	1.00	25.43
326	CZ	PHE	A	36	64.881	50.295	19.910	1.00	26.41
328	CE2	PHE	A	36	64.600	50.022	21.218	1.00	26.08
330	CD2	PHE	A	36	63.624	50.755	21.886	1.00	25.98
332	C	PHE	A	36	59.855	52.427	23.491	1.00	27.72
333	O	PHE	A	36	60.189	52.684	24.642	1.00	27.44
334	N	ILE	A	37	58.679	52.775	22.979	1.00	27.76
336	CA	ILE	A	37	57.677	53.488	23.756	1.00	28.44
338	CB	ILE	A	37	56.779	54.342	22.815	1.00	28.50
340	CG1	ILE	A	37	57.527	55.620	22.419	1.00	28.68
343	CD1	ILE	A	37	56.932	56.377	21.266	1.00	29.67
347	CG2	ILE	A	37	55.440	54.687	23.473	1.00	29.47
351	C	ILE	A	37	56.831	52.526	24.620	1.00	28.85
352	O	ILE	A	37	56.394	52.900	25.707	1.00	29.06
353	N	ALA	A	38	56.631	51.293	24.156	1.00	29.01
355	CA	ALA	A	38	55.688	50.357	24.797	1.00	29.51
357	CB	ALA	A	38	55.489	49.108	23.926	1.00	29.54
361	C	ALA	A	38	55.995	49.951	26.251	1.00	29.76
362	O	ALA	A	38	55.058	49.805	27.032	1.00	30.41
363	N	PRO	A	39	57.261	49.761	26.631	1.00	29.96
364	CA	PRO	A	39	57.590	49.430	28.028	1.00	29.81
366	CB	PRO	A	39	59.019	48.871	27.952	1.00	29.63
369	CG	PRO	A	39	59.465	48.986	26.511	1.00	30.25
372	CD	PRO	A	39	58.466	49.813	25.784	1.00	30.23
375	C	PRO	A	39	57.547	50.605	29.003	1.00	29.35
376	O	PRO	A	39	57.768	50.409	30.200	1.00	29.40
377	N	LEU	A	40	57.288	51.808	28.508	1.00	28.66
379	CA	LEU	A	40	57.243	52.978	29.364	1.00	27.78
381	CB	LEU	A	40	57.200	54.260	28.535	1.00	27.92
384	CG	LEU	A	40	58.410	54.574	27.654	1.00	28.42
386	CD1	LEU	A	40	58.185	55.906	26.946	1.00	29.06
390	CD2	LEU	A	40	59.716	54.573	28.481	1.00	28.93
394	C	LEU	A	40	56.009	52.911	30.243	1.00	27.39
395	O	LEU	A	40	54.962	52.410	29.814	1.00	27.10
396	N	PRO	A	41	56.115	53.412	31.471	1.00	26.65
397	CA	PRO	A	41	54.937	53.506	32.338	1.00	26.24
399	CB	PRO	A	41	55.528	53.818	33.719	1.00	26.42

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
402	CG	PRO A	41		56.887	54.444	33.440	1.00	26.56
405	CD	PRO A	41		57.339	53.909	32.122	1.00	26.41
408	C	PRO A	41		54.017	54.624	31.863	1.00	25.76
409	O	PRO A	41		54.386	55.397	30.977	1.00	25.20
410	N	PHE A	42		52.840	54.706	32.469	1.00	25.70
412	CA	PHE A	42		51.873	55.765	32.212	1.00	25.79
414	CB	PHE A	42		52.479	57.131	32.556	1.00	25.87
417	CG	PHE A	42		53.188	57.147	33.878	1.00	25.55
418	CD1	PHE A	42		52.489	56.876	35.049	1.00	25.97
420	CE1	PHE A	42		53.131	56.864	36.274	1.00	25.51
422	CZ	PHE A	42		54.480	57.116	36.349	1.00	25.34
424	CE2	PHE A	42		55.195	57.379	35.186	1.00	25.76
426	CD2	PHE A	42		54.551	57.383	33.959	1.00	24.78
428	C	PHE A	42		51.323	55.730	30.787	1.00	25.98
429	O	PHE A	42		50.987	56.762	30.226	1.00	25.18
430	N	GLN A	43		51.222	54.528	30.221	1.00	26.46
432	CA	GLN A	43		50.537	54.330	28.942	1.00	27.47
434	CB	GLN A	43		50.502	52.854	28.527	1.00	27.56
437	CG	GLN A	43		51.828	52.229	28.185	1.00	28.72
440	CD	GLN A	43		52.596	52.968	27.106	1.00	30.09
441	OE1	GLN A	43		53.817	53.065	27.187	1.00	32.82
442	NE2	GLN A	43		51.897	53.475	26.096	1.00	30.99
445	C	GLN A	43		49.111	54.786	29.106	1.00	28.28
446	O	GLN A	43		48.511	54.598	30.172	1.00	28.52
447	N	ASN A	44		48.579	55.403	28.060	1.00	28.97
449	CA	ASN A	44		47.202	55.868	28.040	1.00	29.76
451	CB	ASN A	44		46.212	54.687	28.180	1.00	30.31
454	CG	ASN A	44		46.513	53.535	27.210	1.00	31.66
455	OD1	ASN A	44		46.576	53.726	25.997	1.00	36.40
456	ND2	ASN A	44		46.694	52.342	27.748	1.00	32.76
459	C	ASN A	44		46.937	56.948	29.094	1.00	29.56
460	O	ASN A	44		45.842	57.041	29.631	1.00	29.84
461	N	THR A	45		47.958	57.750	29.393	1.00	29.02
463	CA	THR A	45		47.782	59.023	30.090	1.00	28.55
465	CB	THR A	45		48.663	59.090	31.346	1.00	28.99
467	OG1	THR A	45		50.045	59.094	30.966	1.00	29.70
469	CG2	THR A	45		48.504	57.836	32.213	1.00	29.52
473	C	THR A	45		48.173	60.135	29.107	1.00	27.72
474	O	THR A	45		48.886	59.861	28.147	1.00	27.59
475	N	PRO A	46		47.713	61.371	29.316	1.00	26.46
476	CA	PRO A	46		47.961	62.453	28.351	1.00	25.93
478	CB	PRO A	46		47.404	63.699	29.061	1.00	25.92
481	CG	PRO A	46		46.331	63.155	29.974	1.00	26.20
484	CD	PRO A	46		46.879	61.831	30.447	1.00	26.74
487	C	PRO A	46		49.419	62.688	27.918	1.00	25.28
488	O	PRO A	46		49.638	62.912	26.731	1.00	24.82
489	N	VAL A	47		50.389	62.661	28.824	1.00	24.84
491	CA	VAL A	47		51.766	62.944	28.412	1.00	24.49
493	CB	VAL A	47		52.711	63.189	29.616	1.00	24.35
495	CG1	VAL A	47		52.934	61.920	30.414	1.00	25.47
499	CG2	VAL A	47		54.047	63.752	29.131	1.00	25.13
503	C	VAL A	47		52.317	61.860	27.460	1.00	23.84

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
504	O	VAL	A	47	52.962	62.172	26.462	1.00	23.42
505	N	VAL	A	48	52.046	60.594	27.752	1.00	23.38
507	CA	VAL	A	48	52.505	59.516	26.878	1.00	23.48
509	CB	VAL	A	48	52.449	58.146	27.567	1.00	23.07
511	CG1	VAL	A	48	52.773	57.012	26.566	1.00	23.03
515	CG2	VAL	A	48	53.409	58.125	28.740	1.00	23.55
519	C	VAL	A	48	51.725	59.512	25.567	1.00	23.67
520	O	VAL	A	48	52.297	59.299	24.510	1.00	23.73
521	N	GLU	A	49	50.427	59.782	25.632	1.00	23.99
523	CA	GLU	A	49	49.629	59.897	24.417	1.00	24.17
525	CB	GLU	A	49	48.155	60.087	24.761	1.00	24.86
528	CG	GLU	A	49	47.534	58.863	25.404	1.00	27.67
531	CD	GLU	A	49	46.125	59.115	25.899	1.00	33.01
532	OE1	GLU	A	49	45.337	58.140	25.909	1.00	36.58
533	OE2	GLU	A	49	45.806	60.274	26.278	1.00	35.89
534	C	GLU	A	49	50.115	61.066	23.562	1.00	22.99
535	O	GLU	A	49	50.099	60.980	22.345	1.00	21.91
536	N	THR	A	50	50.574	62.139	24.208	1.00	22.14
538	CA	THR	A	50	51.147	63.270	23.497	1.00	21.71
540	CB	THR	A	50	51.426	64.447	24.442	1.00	21.87
542	OG1	THR	A	50	50.218	64.833	25.112	1.00	21.63
544	CG2	THR	A	50	51.861	65.695	23.647	1.00	21.55
548	C	THR	A	50	52.435	62.833	22.813	1.00	21.19
549	O	THR	A	50	52.658	63.152	21.667	1.00	20.77
550	N	MET	A	51	53.268	62.075	23.515	1.00	21.45
552	CA	MET	A	51	54.525	61.583	22.936	1.00	21.16
554	CB	MET	A	51	55.321	60.768	23.965	1.00	21.28
557	CG	MET	A	51	55.825	61.558	25.165	1.00	21.06
560	SD	MET	A	51	56.503	60.485	26.448	1.00	21.92
561	CE	MET	A	51	58.036	59.941	25.581	1.00	18.94
565	C	MET	A	51	54.227	60.713	21.704	1.00	21.05
566	O	MET	A	51	54.873	60.858	20.676	1.00	21.01
567	N	GLN	A	52	53.228	59.835	21.812	1.00	21.04
569	CA	GLN	A	52	52.882	58.908	20.737	1.00	21.29
571	CB	GLN	A	52	51.862	57.889	21.229	1.00	21.77
574	CG	GLN	A	52	52.407	56.822	22.155	1.00	23.17
577	CD	GLN	A	52	51.297	55.954	22.728	1.00	26.61
578	OE1	GLN	A	52	51.254	54.743	22.480	1.00	30.25
579	NE2	GLN	A	52	50.389	56.569	23.474	1.00	24.83
582	C	GLN	A	52	52.299	59.642	19.526	1.00	21.06
583	O	GLN	A	52	52.547	59.291	18.371	1.00	19.85
584	N	TYR	A	53	51.495	60.656	19.804	1.00	20.82
586	CA	TYR	A	53	50.887	61.466	18.760	1.00	21.28
588	CB	TYR	A	53	49.946	62.447	19.433	1.00	21.43
591	CG	TYR	A	53	49.135	63.357	18.555	1.00	23.00
592	CD1	TYR	A	53	47.838	63.002	18.154	1.00	24.56
594	CE1	TYR	A	53	47.069	63.859	17.385	1.00	24.49
596	CZ	TYR	A	53	47.562	65.107	17.052	1.00	25.48
597	OH	TYR	A	53	46.793	65.965	16.292	1.00	24.53
599	CE2	TYR	A	53	48.844	65.484	17.445	1.00	23.07
601	CD2	TYR	A	53	49.604	64.618	18.212	1.00	23.55
603	C	TYR	A	53	51.967	62.218	18.002	1.00	20.79

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
604	O	TYR	A	53	52.033	62.184	16.765	1.00	20.35
605	N	GLY	A	54	52.811	62.910	18.761	1.00	20.69
607	CA	GLY	A	54	53.840	63.751	18.187	1.00	20.90
610	C	GLY	A	54	54.963	62.972	17.526	1.00	21.30
611	O	GLY	A	54	55.596	63.495	16.627	1.00	21.54
612	N	ALA	A	55	55.215	61.732	17.955	1.00	21.95
614	CA	ALA	A	55	56.315	60.942	17.389	1.00	22.16
616	CB	ALA	A	55	56.981	60.100	18.480	1.00	22.04
620	C	ALA	A	55	55.862	60.033	16.242	1.00	22.84
621	O	ALA	A	55	56.609	59.808	15.282	1.00	22.77
622	N	LEU	A	56	54.645	59.506	16.337	1.00	23.82
624	CA	LEU	A	56	54.227	58.413	15.446	1.00	25.01
626	CB	LEU	A	56	53.718	57.229	16.272	1.00	25.40
629	CG	LEU	A	56	54.803	56.448	16.999	1.00	26.02
631	CD1	LEU	A	56	54.192	55.617	18.110	1.00	27.58
635	CD2	LEU	A	56	55.583	55.570	16.011	1.00	26.63
639	C	LEU	A	56	53.188	58.758	14.386	1.00	25.71
640	O	LEU	A	56	53.144	58.088	13.352	1.00	25.79
641	N	LEU	A	57	52.351	59.772	14.626	1.00	26.23
643	CA	LEU	A	57	51.244	60.076	13.712	1.00	26.84
645	CB	LEU	A	57	50.045	60.627	14.487	1.00	27.25
648	CG	LEU	A	57	48.675	60.380	13.836	1.00	29.61
650	CD1	LEU	A	57	48.417	58.886	13.617	1.00	30.97
654	CD2	LEU	A	57	47.544	60.990	14.672	1.00	31.15
658	C	LEU	A	57	51.660	61.041	12.589	1.00	26.56
659	O	LEU	A	57	51.650	62.260	12.762	1.00	26.92
660	N	GLY	A	58	52.014	60.471	11.441	1.00	26.04
662	CA	GLY	A	58	52.480	61.230	10.294	1.00	25.24
665	C	GLY	A	58	53.983	61.421	10.347	1.00	24.44
666	O	GLY	A	58	54.635	61.015	11.301	1.00	24.64
667	N	GLY	A	59	54.513	62.081	9.331	1.00	23.73
669	CA	GLY	A	59	55.938	62.322	9.195	1.00	23.06
672	C	GLY	A	59	56.553	61.359	8.209	1.00	22.26
673	O	GLY	A	59	56.162	60.194	8.133	1.00	22.42
674	N	LYS	A	60	57.547	61.842	7.478	1.00	22.13
676	CA	LYS	A	60	58.154	61.112	6.374	1.00	21.99
678	CB	LYS	A	60	58.759	62.101	5.373	1.00	22.38
681	CG	LYS	A	60	57.740	63.053	4.741	1.00	22.42
684	CD	LYS	A	60	58.397	63.946	3.700	1.00	22.36
687	CE	LYS	A	60	59.309	65.000	4.315	1.00	22.65
690	NZ	LYS	A	60	58.610	65.764	5.390	1.00	22.32
694	C	LYS	A	60	59.236	60.121	6.820	1.00	21.22
695	O	LYS	A	60	59.639	59.250	6.044	1.00	21.45
696	N	ARG	A	61	59.679	60.268	8.064	1.00	20.48
698	CA	ARG	A	61	60.763	59.494	8.657	1.00	19.82
700	CB	ARG	A	61	60.347	58.035	8.877	1.00	19.66
703	CG	ARG	A	61	59.138	57.855	9.723	1.00	20.10
706	CD	ARG	A	61	59.272	58.230	11.192	1.00	20.40
709	NE	ARG	A	61	57.948	58.049	11.781	1.00	20.92
711	CZ	ARG	A	61	57.037	58.991	11.934	1.00	22.13
712	NH1	ARG	A	61	57.298	60.255	11.645	1.00	23.06
715	NH2	ARG	A	61	55.840	58.667	12.421	1.00	22.86

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
718	C	ARG	A	61	62.061	59.514	7.860	1.00	19.24
719	O	ARG	A	61	62.738	58.501	7.779	1.00	18.48
720	N	LEU	A	62	62.432	60.666	7.307	1.00	18.87
722	CA	LEU	A	62	63.630	60.734	6.485	1.00	18.40
724	CB	LEU	A	62	63.643	61.988	5.629	1.00	18.86
727	CG	LEU	A	62	62.430	62.083	4.708	1.00	18.30
729	CD1	LEU	A	62	62.550	63.320	3.821	1.00	18.04
733	CD2	LEU	A	62	62.266	60.815	3.896	1.00	19.13
737	C	LEU	A	62	64.908	60.646	7.296	1.00	18.46
738	O	LEU	A	62	65.933	60.241	6.772	1.00	18.88
739	N	ARG	A	63	64.866	61.017	8.562	1.00	17.65
741	CA	ARG	A	63	66.054	60.871	9.384	1.00	17.87
743	CB	ARG	A	63	66.000	61.756	10.611	1.00	17.85
746	CG	ARG	A	63	66.045	63.219	10.223	1.00	17.38
749	CD	ARG	A	63	65.459	64.177	11.253	1.00	17.84
752	NE	ARG	A	63	65.361	65.533	10.704	1.00	19.01
754	CZ	ARG	A	63	64.417	65.941	9.863	1.00	20.05
755	NH1	ARG	A	63	64.422	67.193	9.411	1.00	22.90
758	NH2	ARG	A	63	63.449	65.123	9.477	1.00	21.09
761	C	ARG	A	63	66.322	59.401	9.705	1.00	17.71
762	O	ARG	A	63	67.454	58.951	9.531	1.00	18.10
763	N	PRO	A	64	65.329	58.645	10.163	1.00	17.51
764	CA	PRO	A	64	65.476	57.180	10.192	1.00	17.45
766	CB	PRO	A	64	64.070	56.703	10.531	1.00	17.56
769	CG	PRO	A	64	63.506	57.791	11.356	1.00	17.73
772	CD	PRO	A	64	64.052	59.064	10.767	1.00	17.18
775	C	PRO	A	64	65.936	56.615	8.859	1.00	17.33
776	O	PRO	A	64	66.816	55.755	8.854	1.00	17.25
777	N	PHE	A	65	65.376	57.104	7.754	1.00	17.93
779	CA	PHE	A	65	65.781	56.677	6.427	1.00	18.40
781	CB	PHE	A	65	65.044	57.457	5.338	1.00	19.10
784	CG	PHE	A	65	65.198	56.872	3.941	1.00	19.82
785	CD1	PHE	A	65	66.425	56.898	3.278	1.00	21.48
787	CE1	PHE	A	65	66.558	56.356	1.990	1.00	24.16
789	CZ	PHE	A	65	65.456	55.801	1.354	1.00	23.70
791	CE2	PHE	A	65	64.232	55.787	2.000	1.00	24.40
793	CD2	PHE	A	65	64.112	56.329	3.289	1.00	21.85
795	C	PHE	A	65	67.288	56.831	6.274	1.00	18.39
796	O	PHE	A	65	67.951	55.920	5.814	1.00	18.40
797	N	LEU	A	66	67.820	57.973	6.683	1.00	18.52
799	CA	LEU	A	66	69.255	58.228	6.643	1.00	18.77
801	CB	LEU	A	66	69.554	59.650	7.101	1.00	19.16
804	CG	LEU	A	66	69.280	60.737	6.070	1.00	20.56
806	CD1	LEU	A	66	69.409	62.108	6.739	1.00	21.70
810	CD2	LEU	A	66	70.233	60.611	4.897	1.00	21.14
814	C	LEU	A	66	70.063	57.274	7.512	1.00	18.22
815	O	LEU	A	66	71.162	56.862	7.131	1.00	17.84
816	N	VAL	A	67	69.546	56.973	8.693	1.00	16.88
818	CA	VAL	A	67	70.235	56.066	9.609	1.00	17.06
820	CB	VAL	A	67	69.512	56.001	10.969	1.00	16.98
822	CG1	VAL	A	67	70.075	54.909	11.865	1.00	17.14
826	CG2	VAL	A	67	69.621	57.337	11.679	1.00	16.69

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
830	C	VAL	A	67	70.315	54.667	8.984	1.00	17.43
831	O	VAL	A	67	71.391	54.087	8.924	1.00	16.85
832	N	TYR	A	68	69.171	54.175	8.504	1.00	17.82
834	CA	TYR	A	68	69.049	52.853	7.890	1.00	18.73
836	CB	TYR	A	68	67.590	52.546	7.534	1.00	18.65
839	CG	TYR	A	68	66.682	52.294	8.706	1.00	17.77
840	CD1	TYR	A	68	66.993	51.343	9.670	1.00	18.53
842	CE1	TYR	A	68	66.152	51.109	10.734	1.00	19.24
844	CZ	TYR	A	68	64.967	51.819	10.844	1.00	17.86
845	OH	TYR	A	68	64.123	51.616	11.915	1.00	16.87
847	CE2	TYR	A	68	64.650	52.774	9.914	1.00	18.34
849	CD2	TYR	A	68	65.492	52.988	8.835	1.00	18.14
851	C	TYR	A	68	69.878	52.741	6.626	1.00	19.22
852	O	TYR	A	68	70.627	51.788	6.466	1.00	20.65
853	N	ALA	A	69	69.762	53.725	5.744	1.00	19.41
855	CA	ALA	A	69	70.470	53.707	4.474	1.00	19.53
857	CB	ALA	A	69	70.035	54.875	3.616	1.00	20.02
861	C	ALA	A	69	71.975	53.744	4.695	1.00	20.18
862	O	ALA	A	69	72.721	53.053	4.011	1.00	21.39
863	N	THR	A	70	72.423	54.545	5.656	1.00	20.00
865	CA	THR	A	70	73.841	54.656	5.930	1.00	20.26
867	CB	THR	A	70	74.124	55.842	6.828	1.00	20.06
869	OG1	THR	A	70	73.742	57.060	6.143	1.00	19.95
871	CG2	THR	A	70	75.624	55.979	7.077	1.00	20.73
875	C	THR	A	70	74.371	53.370	6.527	1.00	20.27
876	O	THR	A	70	75.330	52.821	6.025	1.00	20.97
877	N	GLY	A	71	73.743	52.886	7.588	1.00	20.36
879	CA	GLY	A	71	74.136	51.630	8.199	1.00	20.44
882	C	GLY	A	71	74.090	50.470	7.229	1.00	20.43
883	O	GLY	A	71	74.966	49.600	7.242	1.00	21.38
884	N	HIS	A	72	73.061	50.442	6.393	1.00	21.26
886	CA	HIS	A	72	72.886	49.367	5.401	1.00	21.95
888	CB	HIS	A	72	71.577	49.530	4.623	1.00	22.16
891	CG	HIS	A	72	70.369	49.049	5.362	1.00	21.95
892	ND1	HIS	A	72	69.094	49.468	5.051	1.00	23.29
894	CE1	HIS	A	72	68.231	48.892	5.869	1.00	23.63
896	NE2	HIS	A	72	68.899	48.097	6.687	1.00	21.16
898	CD2	HIS	A	72	70.238	48.181	6.394	1.00	22.72
900	C	HIS	A	72	74.054	49.313	4.421	1.00	22.56
901	O	HIS	A	72	74.455	48.228	3.995	1.00	21.64
902	N	MET	A	73	74.610	50.477	4.080	1.00	23.05
904	CA	MET	A	73	75.782	50.536	3.201	1.00	23.89
906	CB	MET	A	73	76.282	51.961	3.027	1.00	24.12
909	CG	MET	A	73	75.546	52.765	2.016	1.00	26.38
912	SD	MET	A	73	76.590	54.090	1.347	1.00	31.06
913	CE	MET	A	73	77.179	54.849	2.837	1.00	30.61
917	C	MET	A	73	76.944	49.713	3.732	1.00	24.04
918	O	MET	A	73	77.740	49.208	2.945	1.00	24.70
919	N	PHE	A	74	77.052	49.617	5.057	1.00	24.12
921	CA	PHE	A	74	78.122	48.863	5.723	1.00	24.15
923	CB	PHE	A	74	78.644	49.693	6.881	1.00	24.28
926	CG	PHE	A	74	79.127	51.040	6.455	1.00	25.09

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
927	CD1	PHE	A	74	78.410	52.183	6.759	1.00	25.88
929	CE1	PHE	A	74	78.847	53.424	6.357	1.00	25.67
931	CZ	PHE	A	74	80.015	53.547	5.641	1.00	26.11
933	CE2	PHE	A	74	80.751	52.415	5.330	1.00	26.51
935	CD2	PHE	A	74	80.305	51.167	5.736	1.00	26.10
937	C	PHE	A	74	77.710	47.461	6.196	1.00	24.09
938	O	PHE	A	74	78.475	46.770	6.875	1.00	23.88
939	N	GLY	A	75	76.508	47.039	5.815	1.00	23.45
941	CA	GLY	A	75	76.025	45.708	6.114	1.00	23.38
944	C	GLY	A	75	75.544	45.539	7.545	1.00	23.11
945	O	GLY	A	75	75.412	44.415	8.032	1.00	22.14
946	N	VAL	A	76	75.261	46.636	8.241	1.00	22.50
948	CA	VAL	A	76	74.698	46.461	9.577	1.00	22.69
950	CB	VAL	A	76	75.093	47.576	10.642	1.00	22.92
952	CG1	VAL	A	76	75.915	48.711	10.067	1.00	23.76
956	CG2	VAL	A	76	73.908	48.074	11.396	1.00	22.71
960	C	VAL	A	76	73.194	46.144	9.484	1.00	21.96
961	O	VAL	A	76	72.487	46.604	8.591	1.00	21.42
962	N	SER	A	77	72.746	45.302	10.402	1.00	21.48
964	CA	SER	A	77	71.389	44.778	10.405	1.00	21.77
966	CB	SER	A	77	71.250	43.671	11.467	1.00	22.01
969	OG	SER	A	77	69.901	43.269	11.656	1.00	24.55
971	C	SER	A	77	70.388	45.893	10.669	1.00	21.66
972	O	SER	A	77	70.614	46.768	11.497	1.00	20.52
973	N	THR	A	78	69.280	45.849	9.950	1.00	21.30
975	CA	THR	A	78	68.197	46.782	10.145	1.00	21.37
977	CB	THR	A	78	67.041	46.395	9.243	1.00	21.59
979	OG1	THR	A	78	67.522	46.238	7.898	1.00	20.65
981	CG2	THR	A	78	66.004	47.531	9.175	1.00	21.88
985	C	THR	A	78	67.742	46.839	11.609	1.00	21.40
986	O	THR	A	78	67.457	47.919	12.127	1.00	20.26
987	N	ASN	A	79	67.712	45.681	12.273	1.00	20.85
989	CA	ASN	A	79	67.259	45.592	13.665	1.00	21.11
991	CB	ASN	A	79	67.155	44.113	14.110	1.00	20.78
994	CG	ASN	A	79	66.777	43.962	15.577	1.00	20.57
995	OD1	ASN	A	79	65.629	44.176	15.960	1.00	20.74
996	ND2	ASN	A	79	67.741	43.572	16.395	1.00	21.96
999	C	ASN	A	79	68.135	46.366	14.648	1.00	21.18
1000	O	ASN	A	79	67.630	46.935	15.589	1.00	21.24
1001	N	THR	A	80	69.445	46.363	14.445	1.00	21.31
1003	CA	THR	A	80	70.325	47.176	15.288	1.00	22.18
1005	CB	THR	A	80	71.831	46.719	15.233	1.00	23.07
1007	OG1	THR	A	80	72.729	47.845	15.254	1.00	25.14
1009	CG2	THR	A	80	72.163	46.051	13.972	1.00	25.36
1013	C	THR	A	80	70.149	48.653	14.952	1.00	21.28
1014	O	THR	A	80	70.191	49.488	15.836	1.00	21.18
1015	N	LEU	A	81	69.889	48.958	13.685	1.00	20.13
1017	CA	LEU	A	81	69.699	50.338	13.267	1.00	19.67
1019	CB	LEU	A	81	69.773	50.458	11.743	1.00	19.03
1022	CG	LEU	A	81	71.174	50.220	11.203	1.00	20.05
1024	CD1	LEU	A	81	71.133	49.777	9.747	1.00	20.55
1028	CD2	LEU	A	81	72.025	51.477	11.362	1.00	21.66

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1032	C	LEU	A	81	68.395	50.943	13.785	1.00	19.10
1033	O	LEU	A	81	68.266	52.154	13.797	1.00	17.73
1034	N	ASP	A	82	67.452	50.098	14.213	1.00	18.92
1036	CA	ASP	A	82	66.206	50.555	14.808	1.00	19.26
1038	CB	ASP	A	82	65.374	49.380	15.347	1.00	19.80
1041	CG	ASP	A	82	64.537	48.689	14.279	1.00	21.07
1042	OD1	ASP	A	82	64.370	49.232	13.167	1.00	22.88
1043	OD2	ASP	A	82	63.977	47.584	14.496	1.00	22.05
1044	C	ASP	A	82	66.491	51.503	15.972	1.00	18.72
1045	O	ASP	A	82	65.743	52.455	16.193	1.00	18.90
1046	N	ALA	A	83	67.551	51.227	16.724	1.00	18.47
1048	CA	ALA	A	83	67.879	52.031	17.902	1.00	18.05
1050	CB	ALA	A	83	68.957	51.350	18.777	1.00	18.08
1054	C	ALA	A	83	68.262	53.464	17.528	1.00	17.75
1055	O	ALA	A	83	67.571	54.391	17.954	1.00	16.58
1056	N	PRO	A	84	69.334	53.674	16.754	1.00	17.46
1057	CA	PRO	A	84	69.660	55.034	16.310	1.00	17.24
1059	CB	PRO	A	84	70.978	54.870	15.537	1.00	17.48
1062	CG	PRO	A	84	71.073	53.397	15.176	1.00	17.90
1065	CD	PRO	A	84	70.318	52.690	16.274	1.00	17.39
1068	C	PRO	A	84	68.570	55.674	15.452	1.00	17.54
1069	O	PRO	A	84	68.372	56.871	15.546	1.00	16.99
1070	N	ALA	A	85	67.881	54.899	14.617	1.00	17.55
1072	CA	ALA	A	85	66.786	55.439	13.827	1.00	17.51
1074	CB	ALA	A	85	66.196	54.371	12.908	1.00	17.15
1078	C	ALA	A	85	65.710	56.010	14.751	1.00	17.33
1079	O	ALA	A	85	65.235	57.120	14.540	1.00	17.48
1080	N	ALA	A	86	65.365	55.276	15.797	1.00	17.28
1082	CA	ALA	A	86	64.309	55.702	16.702	1.00	17.98
1084	CB	ALA	A	86	63.858	54.558	17.575	1.00	17.95
1088	C	ALA	A	86	64.764	56.881	17.559	1.00	18.07
1089	O	ALA	A	86	63.986	57.800	17.828	1.00	18.55
1090	N	ALA	A	87	66.027	56.852	17.965	1.00	17.63
1092	CA	ALA	A	87	66.612	57.905	18.776	1.00	17.90
1094	CB	ALA	A	87	68.016	57.551	19.129	1.00	17.89
1098	C	ALA	A	87	66.602	59.238	18.046	1.00	18.01
1099	O	ALA	A	87	66.199	60.258	18.611	1.00	16.96
1100	N	VAL	A	88	67.076	59.233	16.802	1.00	18.36
1102	CA	VAL	A	88	67.108	60.469	16.022	1.00	19.02
1104	CB	VAL	A	88	67.919	60.359	14.706	1.00	19.48
1106	CG1	VAL	A	88	69.346	59.943	15.004	1.00	21.38
1110	CG2	VAL	A	88	67.262	59.431	13.694	1.00	20.88
1114	C	VAL	A	88	65.697	60.984	15.728	1.00	18.91
1115	O	VAL	A	88	65.478	62.192	15.694	1.00	19.41
1116	N	GLU	A	89	64.755	60.075	15.506	1.00	18.77
1118	CA	GLU	A	89	63.371	60.460	15.281	1.00	19.03
1120	CB	GLU	A	89	62.580	59.307	14.672	1.00	19.35
1123	CG	GLU	A	89	61.202	59.659	14.140	1.00	20.47
1126	CD	GLU	A	89	61.187	60.686	13.014	1.00	23.08
1127	OE1	GLU	A	89	60.085	61.188	12.699	1.00	21.79
1128	OE2	GLU	A	89	62.243	61.001	12.436	1.00	22.95
1129	C	GLU	A	89	62.726	60.972	16.571	1.00	19.06

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1130	O	GLU	A	89	61.883	61.856	16.515	1.00	18.98
1131	N	CYS	A	90	63.154	60.466	17.724	1.00	19.07
1133	CA	CYS	A	90	62.684	61.026	18.999	1.00	19.48
1135	CB	CYS	A	90	63.154	60.218	20.204	1.00	19.62
1138	SG	CYS	A	90	62.240	58.692	20.462	1.00	21.40
1139	C	CYS	A	90	63.139	62.464	19.144	1.00	18.83
1140	O	CYS	A	90	62.348	63.311	19.526	1.00	19.11
1141	N	ILE	A	91	64.405	62.740	18.846	1.00	18.13
1143	CA	ILE	A	91	64.900	64.108	18.934	1.00	17.94
1145	CB	ILE	A	91	66.402	64.201	18.602	1.00	18.00
1147	CG1	ILE	A	91	67.269	63.442	19.628	1.00	18.23
1150	CD1	ILE	A	91	67.160	63.942	21.057	1.00	18.91
1154	CG2	ILE	A	91	66.824	65.659	18.520	1.00	18.94
1158	C	ILE	A	91	64.117	64.994	17.959	1.00	17.15
1159	O	ILE	A	91	63.700	66.094	18.308	1.00	16.79
1160	N	HIS	A	92	63.952	64.506	16.732	1.00	16.32
1162	CA	HIS	A	92	63.238	65.238	15.701	1.00	16.58
1164	CB	HIS	A	92	63.182	64.438	14.409	1.00	16.65
1167	CG	HIS	A	92	62.424	65.119	13.321	1.00	16.27
1168	ND1	HIS	A	92	61.352	64.536	12.675	1.00	17.53
1170	CE1	HIS	A	92	60.892	65.378	11.761	1.00	15.88
1172	NE2	HIS	A	92	61.620	66.480	11.800	1.00	17.29
1174	CD2	HIS	A	92	62.573	66.348	12.779	1.00	15.01
1176	C	HIS	A	92	61.825	65.555	16.167	1.00	16.53
1177	O	HIS	A	92	61.399	66.712	16.151	1.00	16.57
1178	N	ALA	A	93	61.119	64.532	16.620	1.00	15.86
1180	CA	ALA	A	93	59.753	64.699	17.119	1.00	16.23
1182	CB	ALA	A	93	59.177	63.346	17.566	1.00	16.25
1186	C	ALA	A	93	59.671	65.720	18.251	1.00	16.36
1187	O	ALA	A	93	58.753	66.544	18.297	1.00	16.22
1188	N	TYR	A	94	60.632	65.668	19.168	1.00	16.81
1190	CA	TYR	A	94	60.653	66.585	20.289	1.00	17.25
1192	CB	TYR	A	94	61.742	66.187	21.312	1.00	18.09
1195	CG	TYR	A	94	62.785	67.233	21.639	1.00	18.65
1196	CD1	TYR	A	94	62.444	68.391	22.309	1.00	20.51
1198	CE1	TYR	A	94	63.388	69.341	22.613	1.00	22.48
1200	CZ	TYR	A	94	64.701	69.138	22.248	1.00	22.20
1201	OH	TYR	A	94	65.628	70.083	22.565	1.00	24.51
1203	CE2	TYR	A	94	65.075	67.983	21.590	1.00	21.60
1205	CD2	TYR	A	94	64.122	67.037	21.306	1.00	19.95
1207	C	TYR	A	94	60.837	68.001	19.766	1.00	17.28
1208	O	TYR	A	94	60.178	68.921	20.232	1.00	16.91
1209	N	SER	A	95	61.709	68.169	18.780	1.00	17.12
1211	CA	SER	A	95	62.028	69.486	18.281	1.00	17.61
1213	CB	SER	A	95	63.209	69.446	17.312	1.00	17.91
1216	OG	SER	A	95	62.859	68.946	16.045	1.00	19.03
1218	C	SER	A	95	60.787	70.161	17.665	1.00	18.18
1219	O	SER	A	95	60.591	71.367	17.826	1.00	17.08
1220	N	LEU	A	96	59.936	69.376	17.021	1.00	18.08
1222	CA	LEU	A	96	58.748	69.937	16.356	1.00	18.75
1224	CB	LEU	A	96	58.168	68.946	15.359	1.00	18.81
1227	CG	LEU	A	96	59.159	68.371	14.350	1.00	19.61

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1229	CD1	LEU	A	96	58.421	67.472	13.385	1.00	19.87
1233	CD2	LEU	A	96	59.901	69.477	13.628	1.00	20.82
1237	C	LEU	A	96	57.676	70.285	17.371	1.00	18.79
1238	O	LEU	A	96	56.928	71.252	17.192	1.00	19.67
1239	N	ILE	A	97	57.581	69.478	18.422	1.00	18.80
1241	CA	ILE	A	97	56.574	69.704	19.448	1.00	18.69
1243	CB	ILE	A	97	56.590	68.612	20.520	1.00	18.23
1245	CG1	ILE	A	97	56.062	67.307	19.941	1.00	17.66
1248	CD1	ILE	A	97	56.017	66.149	20.924	1.00	19.38
1252	CG2	ILE	A	97	55.756	69.050	21.746	1.00	18.51
1256	C	ILE	A	97	56.844	71.069	20.071	1.00	19.44
1257	O	ILE	A	97	55.925	71.851	20.233	1.00	19.55
1258	N	HIS	A	98	58.108	71.358	20.383	1.00	19.42
1260	CA	HIS	A	98	58.452	72.609	21.039	1.00	20.66
1262	CB	HIS	A	98	59.797	72.507	21.730	1.00	21.50
1265	CG	HIS	A	98	59.735	71.795	23.045	1.00	25.90
1266	ND1	HIS	A	98	59.610	70.432	23.149	1.00	34.19
1268	CE1	HIS	A	98	59.570	70.087	24.425	1.00	32.41
1270	NE2	HIS	A	98	59.660	71.175	25.149	1.00	32.34
1272	CD2	HIS	A	98	59.748	72.261	24.312	1.00	32.88
1274	C	HIS	A	98	58.437	73.774	20.072	1.00	20.22
1275	O	HIS	A	98	58.095	74.880	20.444	1.00	20.04
1276	N	ASP	A	99	58.809	73.500	18.829	1.00	20.34
1278	CA	ASP	A	99	58.834	74.488	17.772	1.00	20.27
1280	CB	ASP	A	99	59.394	73.845	16.496	1.00	20.14
1283	CG	ASP	A	99	59.438	74.806	15.326	1.00	19.89
1284	OD1	ASP	A	99	58.542	74.720	14.458	1.00	20.18
1285	OD2	ASP	A	99	60.332	75.665	15.194	1.00	18.02
1286	C	ASP	A	99	57.447	75.081	17.512	1.00	20.91
1287	O	ASP	A	99	57.322	76.277	17.253	1.00	21.26
1288	N	ASP	A	100	56.410	74.254	17.580	1.00	21.41
1290	CA	ASP	A	100	55.037	74.718	17.328	1.00	21.41
1292	CB	ASP	A	100	54.098	73.551	17.048	1.00	21.45
1295	CG	ASP	A	100	54.436	72.819	15.799	1.00	20.29
1296	OD1	ASP	A	100	54.167	71.594	15.734	1.00	20.18
1297	OD2	ASP	A	100	54.978	73.379	14.841	1.00	19.29
1298	C	ASP	A	100	54.428	75.500	18.483	1.00	21.71
1299	O	ASP	A	100	53.395	76.123	18.301	1.00	22.06
1300	N	LEU	A	101	55.039	75.467	19.664	1.00	21.73
1302	CA	LEU	A	101	54.463	76.129	20.837	1.00	21.71
1304	CB	LEU	A	101	55.389	76.027	22.052	1.00	21.29
1307	CG	LEU	A	101	55.643	74.639	22.631	1.00	21.02
1309	CD1	LEU	A	101	56.681	74.748	23.744	1.00	21.63
1313	CD2	LEU	A	101	54.375	73.987	23.130	1.00	21.37
1317	C	LEU	A	101	54.173	77.611	20.587	1.00	22.13
1318	O	LEU	A	101	54.852	78.255	19.795	1.00	21.48
1319	N	PRO	A	102	53.167	78.152	21.273	1.00	23.19
1320	CA	PRO	A	102	52.850	79.588	21.175	1.00	23.59
1322	CB	PRO	A	102	51.811	79.779	22.282	1.00	24.00
1325	CG	PRO	A	102	51.099	78.464	22.308	1.00	23.90
1328	CD	PRO	A	102	52.216	77.443	22.149	1.00	22.62
1331	C	PRO	A	102	54.045	80.533	21.348	1.00	24.21

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1332	O	PRO	A	102	54.148	81.494	20.599	1.00	25.11
1333	N	ALA	A	103	54.943	80.255	22.285	1.00	24.74
1335	CA	ALA	A	103	56.123	81.094	22.516	1.00	25.23
1337	CB	ALA	A	103	56.753	80.737	23.867	1.00	25.78
1341	C	ALA	A	103	57.176	80.941	21.417	1.00	25.46
1342	O	ALA	A	103	58.093	81.742	21.317	1.00	24.70
1343	N	MET	A	104	57.053	79.879	20.626	1.00	25.19
1345	CA	MET	A	104	57.981	79.590	19.550	1.00	26.00
1347	CB	MET	A	104	58.362	78.109	19.598	1.00	25.79
1350	CG	MET	A	104	58.997	77.719	20.916	1.00	27.52
1353	SD	MET	A	104	60.690	78.194	20.987	1.00	31.55
1354	CE	MET	A	104	61.411	77.093	19.688	1.00	31.97
1358	C	MET	A	104	57.345	79.995	18.207	1.00	25.73
1359	O	MET	A	104	57.213	81.186	17.942	1.00	25.54
1360	N	ASP	A	105	56.937	79.038	17.374	1.00	25.29
1362	CA	ASP	A	105	56.373	79.388	16.061	1.00	25.81
1364	CB	ASP	A	105	56.832	78.419	14.969	1.00	25.24
1367	CG	ASP	A	105	58.319	78.496	14.716	1.00	24.83
1368	OD1	ASP	A	105	58.853	77.642	13.954	1.00	22.09
1369	OD2	ASP	A	105	59.049	79.364	15.253	1.00	25.62
1370	C	ASP	A	105	54.851	79.525	16.069	1.00	25.92
1371	O	ASP	A	105	54.289	80.054	15.126	1.00	26.07
1372	N	ASP	A	106	54.206	79.043	17.125	1.00	26.89
1374	CA	ASP	A	106	52.759	79.211	17.350	1.00	27.69
1376	CB	ASP	A	106	52.419	80.670	17.671	1.00	28.12
1379	CG	ASP	A	106	51.000	80.840	18.202	1.00	29.63
1380	OD1	ASP	A	106	50.458	81.960	18.094	1.00	31.75
1381	OD2	ASP	A	106	50.342	79.911	18.732	1.00	31.76
1382	C	ASP	A	106	51.952	78.715	16.157	1.00	28.05
1383	O	ASP	A	106	51.159	79.450	15.549	1.00	28.01
1384	N	ASP	A	107	52.190	77.456	15.809	1.00	28.07
1386	CA	ASP	A	107	51.534	76.822	14.686	1.00	27.99
1388	CB	ASP	A	107	52.553	76.037	13.855	1.00	28.56
1391	CG	ASP	A	107	53.069	76.830	12.677	1.00	29.78
1392	OD1	ASP	A	107	52.257	77.111	11.774	1.00	33.36
1393	OD2	ASP	A	107	54.255	77.210	12.549	1.00	31.90
1394	C	ASP	A	107	50.478	75.882	15.230	1.00	27.64
1395	O	ASP	A	107	50.693	75.218	16.248	1.00	26.98
1396	N	ASP	A	108	49.334	75.823	14.559	1.00	26.95
1398	CA	ASP	A	108	48.242	74.989	15.031	1.00	26.81
1400	CB	ASP	A	108	46.929	75.778	15.089	1.00	27.66
1403	CG	ASP	A	108	46.453	76.241	13.725	1.00	30.37
1404	OD1	ASP	A	108	45.282	76.700	13.645	1.00	33.61
1405	OD2	ASP	A	108	47.165	76.194	12.690	1.00	32.04
1406	C	ASP	A	108	48.075	73.702	14.236	1.00	25.96
1407	O	ASP	A	108	47.283	72.856	14.631	1.00	25.76
1408	N	LEU	A	109	48.818	73.559	13.136	1.00	25.04
1410	CA	LEU	A	109	48.751	72.367	12.298	1.00	24.85
1412	CB	LEU	A	109	48.106	72.694	10.945	1.00	25.33
1415	CG	LEU	A	109	46.598	72.821	10.810	1.00	26.83
1417	CD1	LEU	A	109	46.260	73.283	9.399	1.00	29.44
1421	CD2	LEU	A	109	45.903	71.492	11.089	1.00	27.95

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1425	C	LEU	A	109	50.144	71.781	12.034	1.00	23.64
1426	O	LEU	A	109	51.094	72.514	11.790	1.00	23.64
1427	N	ARG	A	110	50.237	70.454	12.081	1.00	22.79
1429	CA	ARG	A	110	51.401	69.715	11.603	1.00	22.20
1431	CB	ARG	A	110	52.479	69.644	12.672	1.00	21.90
1434	CG	ARG	A	110	53.742	69.015	12.166	1.00	21.62
1437	CD	ARG	A	110	54.820	68.975	13.195	1.00	21.16
1440	NE	ARG	A	110	55.377	70.290	13.472	1.00	19.55
1442	CZ	ARG	A	110	56.277	70.905	12.721	1.00	21.19
1443	NH1	ARG	A	110	56.740	72.082	13.111	1.00	21.55
1446	NH2	ARG	A	110	56.737	70.355	11.590	1.00	21.98
1449	C	ARG	A	110	50.997	68.301	11.215	1.00	21.87
1450	O	ARG	A	110	50.184	67.686	11.876	1.00	20.97
1451	N	ARG	A	111	51.566	67.807	10.122	1.00	22.79
1453	CA	ARG	A	111	51.237	66.489	9.580	1.00	23.42
1455	CB	ARG	A	111	51.814	65.407	10.477	1.00	23.33
1458	CG	ARG	A	111	53.310	65.424	10.531	1.00	22.10
1461	CD	ARG	A	111	53.841	64.752	11.768	1.00	21.59
1464	NE	ARG	A	111	55.282	64.632	11.726	1.00	21.10
1466	CZ	ARG	A	111	56.009	64.082	12.681	1.00	21.03
1467	NH1	ARG	A	111	55.438	63.576	13.760	1.00	20.75
1470	NH2	ARG	A	111	57.323	64.020	12.544	1.00	22.79
1473	C	ARG	A	111	49.733	66.284	9.374	1.00	24.49
1474	O	ARG	A	111	49.216	65.181	9.528	1.00	24.90
1475	N	GLY	A	112	49.048	67.375	9.037	1.00	25.84
1477	CA	GLY	A	112	47.641	67.363	8.673	1.00	26.45
1480	C	GLY	A	112	46.709	67.432	9.854	1.00	27.01
1481	O	GLY	A	112	45.500	67.383	9.663	1.00	27.66
1482	N	LEU	A	113	47.258	67.574	11.066	1.00	27.18
1484	CA	LEU	A	113	46.478	67.445	12.301	1.00	27.29
1486	CB	LEU	A	113	46.778	66.104	12.965	1.00	27.61
1489	CG	LEU	A	113	46.308	64.849	12.230	1.00	29.25
1491	CD1	LEU	A	113	46.956	63.639	12.826	1.00	29.40
1495	CD2	LEU	A	113	44.799	64.723	12.297	1.00	30.33
1499	C	LEU	A	113	46.783	68.580	13.279	1.00	26.95
1500	O	LEU	A	113	47.781	69.273	13.134	1.00	26.97
1501	N	PRO	A	114	45.911	68.807	14.256	1.00	26.77
1502	CA	PRO	A	114	46.242	69.737	15.341	1.00	26.42
1504	CB	PRO	A	114	45.151	69.465	16.391	1.00	26.39
1507	CG	PRO	A	114	43.997	68.927	15.636	1.00	27.10
1510	CD	PRO	A	114	44.540	68.278	14.377	1.00	27.03
1513	C	PRO	A	114	47.644	69.428	15.902	1.00	25.96
1514	O	PRO	A	114	47.988	68.247	16.088	1.00	25.12
1515	N	THR	A	115	48.433	70.470	16.131	1.00	25.63
1517	CA	THR	A	115	49.730	70.336	16.803	1.00	25.53
1519	CB	THR	A	115	50.478	71.668	16.835	1.00	25.67
1521	OG1	THR	A	115	49.605	72.715	17.288	1.00	26.41
1523	CG2	THR	A	115	50.901	72.085	15.442	1.00	25.77
1527	C	THR	A	115	49.531	69.838	18.228	1.00	25.27
1528	O	THR	A	115	48.430	69.941	18.787	1.00	24.78
1529	N	CYS	A	116	50.600	69.305	18.817	1.00	24.89
1531	CA	CYS	A	116	50.523	68.697	20.137	1.00	24.95

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1533	CB	CYS	A	116	51.895	68.165	20.581	1.00	24.90
1536	SG	CYS	A	116	52.285	66.565	19.821	1.00	24.91
1537	C	CYS	A	116	49.933	69.634	21.182	1.00	24.97
1538	O	CYS	A	116	49.096	69.228	21.971	1.00	24.71
1539	N	HIS	A	117	50.346	70.894	21.168	1.00	25.78
1541	CA	HIS	A	117	49.925	71.820	22.208	1.00	26.16
1543	CB	HIS	A	117	50.836	73.054	22.246	1.00	26.51
1546	CG	HIS	A	117	50.548	74.067	21.186	1.00	27.10
1547	ND1	HIS	A	117	50.785	73.840	19.849	1.00	30.89
1549	CE1	HIS	A	117	50.441	74.911	19.156	1.00	30.52
1551	NE2	HIS	A	117	50.007	75.831	19.996	1.00	30.35
1553	CD2	HIS	A	117	50.066	75.327	21.272	1.00	29.44
1555	C	HIS	A	117	48.433	72.162	22.054	1.00	26.69
1556	O	HIS	A	117	47.747	72.385	23.040	1.00	26.52
1557	N	VAL	A	118	47.938	72.180	20.820	1.00	27.17
1559	CA	VAL	A	118	46.510	72.380	20.577	1.00	27.86
1561	CB	VAL	A	118	46.217	72.617	19.078	1.00	27.70
1563	CG1	VAL	A	118	44.701	72.510	18.774	1.00	28.86
1567	CG2	VAL	A	118	46.737	73.972	18.645	1.00	28.14
1571	C	VAL	A	118	45.695	71.196	21.131	1.00	28.24
1572	O	VAL	A	118	44.784	71.396	21.935	1.00	28.47
1573	N	LYS	A	119	46.040	69.973	20.733	1.00	28.54
1575	CA	LYS	A	119	45.245	68.798	21.101	1.00	29.34
1577	CB	LYS	A	119	45.617	67.583	20.241	1.00	29.61
1580	CG	LYS	A	119	44.863	66.301	20.626	1.00	30.82
1583	CD	LYS	A	119	45.106	65.186	19.627	1.00	32.53
1586	CE	LYS	A	119	44.199	63.976	19.839	1.00	33.76
1589	NZ	LYS	A	119	43.344	64.050	21.054	1.00	36.05
1593	C	LYS	A	119	45.371	68.422	22.581	1.00	29.59
1594	O	LYS	A	119	44.383	68.012	23.194	1.00	29.82
1595	N	PHE	A	120	46.575	68.551	23.146	1.00	28.84
1597	CA	PHE	A	120	46.839	68.108	24.519	1.00	28.62
1599	CB	PHE	A	120	47.984	67.096	24.529	1.00	28.31
1602	CG	PHE	A	120	47.722	65.880	23.711	1.00	27.28
1603	CD1	PHE	A	120	47.055	64.787	24.261	1.00	27.38
1605	CE1	PHE	A	120	46.831	63.631	23.508	1.00	27.16
1607	CZ	PHE	A	120	47.271	63.563	22.198	1.00	27.58
1609	CE2	PHE	A	120	47.932	64.648	21.636	1.00	27.23
1611	CD2	PHE	A	120	48.163	65.804	22.399	1.00	27.44
1613	C	PHE	A	120	47.185	69.217	25.515	1.00	28.26
1614	O	PHE	A	120	47.341	68.943	26.706	1.00	29.25
1615	N	GLY	A	121	47.299	70.452	25.042	1.00	27.60
1617	CA	GLY	A	121	47.659	71.575	25.896	1.00	26.94
1620	C	GLY	A	121	49.155	71.840	25.860	1.00	26.46
1621	O	GLY	A	121	49.958	70.992	25.438	1.00	26.06
1622	N	GLU	A	122	49.536	73.009	26.340	1.00	25.72
1624	CA	GLU	A	122	50.910	73.462	26.248	1.00	25.58
1626	CB	GLU	A	122	51.007	74.958	26.519	1.00	25.87
1629	CG	GLU	A	122	50.483	75.783	25.358	1.00	29.11
1632	CD	GLU	A	122	50.355	77.241	25.698	1.00	33.26
1633	OE1	GLU	A	122	51.247	77.754	26.399	1.00	35.51
1634	OE2	GLU	A	122	49.349	77.861	25.269	1.00	37.97

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1635	C	GLU	A	122	51.798	72.689	27.211	1.00	24.80
1636	O	GLU	A	122	52.899	72.300	26.840	1.00	24.40
1637	N	ALA	A	123	51.320	72.474	28.436	1.00	23.77
1639	CA	ALA	A	123	52.098	71.760	29.447	1.00	23.73
1641	CB	ALA	A	123	51.353	71.711	30.776	1.00	23.98
1645	C	ALA	A	123	52.441	70.343	28.968	1.00	23.81
1646	O	ALA	A	123	53.603	69.943	29.024	1.00	24.19
1647	N	ASN	A	124	51.442	69.609	28.479	1.00	22.86
1649	CA	ASN	A	124	51.654	68.270	27.947	1.00	22.86
1651	CB	ASN	A	124	50.345	67.623	27.491	1.00	23.02
1654	CG	ASN	A	124	49.539	67.041	28.635	1.00	24.68
1655	OD1	ASN	A	124	48.304	67.110	28.640	1.00	27.85
1656	ND2	ASN	A	124	50.220	66.461	29.600	1.00	25.67
1659	C	ASN	A	124	52.631	68.261	26.779	1.00	21.84
1660	O	ASN	A	124	53.428	67.339	26.667	1.00	22.15
1661	N	ALA	A	125	52.543	69.263	25.908	1.00	20.33
1663	CA	ALA	A	125	53.457	69.399	24.788	1.00	20.39
1665	CB	ALA	A	125	52.984	70.529	23.886	1.00	20.63
1669	C	ALA	A	125	54.925	69.621	25.250	1.00	19.95
1670	O	ALA	A	125	55.856	68.974	24.760	1.00	19.97
1671	N	ILE	A	126	55.117	70.509	26.218	1.00	19.41
1673	CA	ILE	A	126	56.434	70.769	26.790	1.00	19.39
1675	CB	ILE	A	126	56.357	71.842	27.880	1.00	19.07
1677	CG1	ILE	A	126	56.032	73.214	27.267	1.00	20.58
1680	CD1	ILE	A	126	55.450	74.180	28.244	1.00	22.11
1684	CG2	ILE	A	126	57.668	71.944	28.623	1.00	19.77
1688	C	ILE	A	126	57.011	69.487	27.378	1.00	19.19
1689	O	ILE	A	126	58.134	69.105	27.069	1.00	18.97
1690	N	LEU	A	127	56.229	68.824	28.211	1.00	18.52
1692	CA	LEU	A	127	56.694	67.637	28.913	1.00	19.19
1694	CB	LEU	A	127	55.716	67.252	30.029	1.00	19.06
1697	CG	LEU	A	127	55.616	68.280	31.166	1.00	20.37
1699	CD1	LEU	A	127	56.961	68.500	31.859	1.00	22.60
1703	CD2	LEU	A	127	54.595	67.820	32.159	1.00	21.48
1707	C	LEU	A	127	56.907	66.470	27.966	1.00	18.53
1708	O	LEU	A	127	57.856	65.723	28.126	1.00	18.41
1709	N	ALA	A	128	56.033	66.320	26.973	1.00	17.92
1711	CA	ALA	A	128	56.179	65.228	26.012	1.00	17.62
1713	CB	ALA	A	128	54.947	65.115	25.104	1.00	17.67
1717	C	ALA	A	128	57.434	65.418	25.168	1.00	17.09
1718	O	ALA	A	128	58.108	64.461	24.828	1.00	17.12
1719	N	GLY	A	129	57.740	66.649	24.807	1.00	16.81
1721	CA	GLY	A	129	58.945	66.914	24.059	1.00	16.96
1724	C	GLY	A	129	60.155	66.651	24.946	1.00	17.30
1725	O	GLY	A	129	61.102	66.022	24.500	1.00	17.59
1726	N	ASP	A	130	60.106	67.121	26.193	1.00	17.16
1728	CA	ASP	A	130	61.139	66.853	27.190	1.00	17.77
1730	CB	ASP	A	130	60.717	67.383	28.562	1.00	18.20
1733	CG	ASP	A	130	60.801	68.881	28.661	1.00	19.18
1734	OD1	ASP	A	130	61.407	69.492	27.759	1.00	21.99
1735	OD2	ASP	A	130	60.295	69.527	29.612	1.00	19.91
1736	C	ASP	A	130	61.410	65.359	27.301	1.00	17.64

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1737	O	ASP	A	130	62.548	64.927	27.230	1.00	17.90
1738	N	ALA	A	131	60.343	64.584	27.447	1.00	17.42
1740	CA	ALA	A	131	60.438	63.146	27.633	1.00	17.39
1742	CB	ALA	A	131	59.098	62.582	28.089	1.00	17.97
1746	C	ALA	A	131	60.910	62.429	26.378	1.00	17.06
1747	O	ALA	A	131	61.576	61.425	26.482	1.00	16.51
1748	N	LEU	A	132	60.525	62.918	25.197	1.00	17.23
1750	CA	LEU	A	132	61.005	62.333	23.947	1.00	17.60
1752	CB	LEU	A	132	60.265	62.904	22.740	1.00	17.59
1755	CG	LEU	A	132	58.930	62.247	22.427	1.00	17.08
1757	CD1	LEU	A	132	58.170	63.044	21.399	1.00	18.87
1761	CD2	LEU	A	132	59.126	60.798	21.970	1.00	18.78
1765	C	LEU	A	132	62.515	62.534	23.779	1.00	17.74
1766	O	LEU	A	132	63.197	61.641	23.297	1.00	17.61
1767	N	GLN	A	133	63.036	63.695	24.185	1.00	17.96
1769	CA	GLN	A	133	64.483	63.926	24.148	1.00	18.23
1771	CB	GLN	A	133	64.894	65.366	24.559	1.00	18.28
1774	CG	GLN	A	133	66.427	65.512	24.520	1.00	19.50
1777	CD	GLN	A	133	67.021	66.816	25.074	1.00	22.38
1778	OE1	GLN	A	133	66.350	67.833	25.237	1.00	19.65
1779	NE2	GLN	A	133	68.322	66.768	25.346	1.00	23.26
1782	C	GLN	A	133	65.165	62.906	25.043	1.00	17.62
1783	O	GLN	A	133	66.132	62.284	24.645	1.00	17.06
1784	N	THR	A	134	64.650	62.736	26.258	1.00	18.05
1786	CA	THR	A	134	65.220	61.790	27.201	1.00	18.07
1788	CB	THR	A	134	64.461	61.797	28.520	1.00	18.89
1790	OG1	THR	A	134	64.445	63.109	29.073	1.00	17.91
1792	CG2	THR	A	134	65.189	60.940	29.551	1.00	18.65
1796	C	THR	A	134	65.165	60.373	26.665	1.00	17.74
1797	O	THR	A	134	66.111	59.615	26.829	1.00	17.70
1798	N	LEU	A	135	64.056	60.037	26.016	1.00	17.32
1800	CA	LEU	A	135	63.863	58.698	25.487	1.00	17.21
1802	CB	LEU	A	135	62.450	58.554	24.899	1.00	16.68
1805	CG	LEU	A	135	62.102	57.160	24.360	1.00	17.14
1807	CD1	LEU	A	135	62.252	56.096	25.413	1.00	17.24
1811	CD2	LEU	A	135	60.691	57.141	23.772	1.00	17.71
1815	C	LEU	A	135	64.934	58.362	24.443	1.00	16.99
1816	O	LEU	A	135	65.396	57.234	24.373	1.00	17.51
1817	N	ALA	A	136	65.311	59.345	23.637	1.00	16.86
1819	CA	ALA	A	136	66.350	59.191	22.640	1.00	16.98
1821	CB	ALA	A	136	66.617	60.525	21.936	1.00	16.96
1825	C	ALA	A	136	67.629	58.656	23.286	1.00	17.44
1826	O	ALA	A	136	68.269	57.772	22.741	1.00	17.77
1827	N	PHE	A	137	67.982	59.193	24.449	1.00	17.78
1829	CA	PHE	A	137	69.179	58.770	25.172	1.00	18.09
1831	CB	PHE	A	137	69.700	59.891	26.062	1.00	18.06
1834	CG	PHE	A	137	70.113	61.073	25.279	1.00	18.66
1835	CD1	PHE	A	137	69.308	62.203	25.215	1.00	17.95
1837	CE1	PHE	A	137	69.672	63.284	24.422	1.00	18.78
1839	CZ	PHE	A	137	70.834	63.241	23.689	1.00	18.81
1841	CE2	PHE	A	137	71.647	62.108	23.742	1.00	19.03
1843	CD2	PHE	A	137	71.277	61.031	24.526	1.00	19.55

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1845	C	PHE	A	137	69.000	57.481	25.944	1.00	17.78
1846	O	PHE	A	137	69.967	56.741	26.093	1.00	19.01
1847	N	SER	A	138	67.783	57.181	26.383	1.00	17.63
1849	CA	SER	A	138	67.480	55.853	26.930	1.00	17.81
1851	CB	SER	A	138	66.064	55.790	27.503	1.00	18.14
1854	OG	SER	A	138	65.998	56.474	28.749	1.00	19.62
1856	C	SER	A	138	67.634	54.788	25.860	1.00	17.61
1857	O	SER	A	138	68.139	53.706	26.127	1.00	17.31
1858	N	ILE	A	139	67.202	55.100	24.646	1.00	17.34
1860	CA	ILE	A	139	67.275	54.150	23.545	1.00	18.07
1862	CB	ILE	A	139	66.528	54.676	22.286	1.00	18.17
1864	CG1	ILE	A	139	65.001	54.638	22.531	1.00	18.76
1867	CD1	ILE	A	139	64.188	55.429	21.499	1.00	19.79
1871	CG2	ILE	A	139	66.878	53.836	21.073	1.00	19.10
1875	C	ILE	A	139	68.732	53.827	23.237	1.00	17.54
1876	O	ILE	A	139	69.102	52.663	23.207	1.00	17.29
1877	N	LEU	A	140	69.556	54.854	23.081	1.00	17.52
1879	CA	LEU	A	140	70.961	54.677	22.710	1.00	18.26
1881	CB	LEU	A	140	71.607	56.028	22.388	1.00	18.48
1884	CG	LEU	A	140	71.151	56.649	21.066	1.00	18.76
1886	CD1	LEU	A	140	71.890	57.952	20.786	1.00	19.92
1890	CD2	LEU	A	140	71.349	55.663	19.939	1.00	19.54
1894	C	LEU	A	140	71.775	53.986	23.786	1.00	18.96
1895	O	LEU	A	140	72.715	53.265	23.476	1.00	18.14
1896	N	SER	A	141	71.414	54.201	25.046	1.00	19.45
1898	CA	SER	A	141	72.165	53.596	26.142	1.00	20.52
1900	CB	SER	A	141	72.125	54.482	27.404	1.00	20.39
1903	OG	SER	A	141	70.812	54.763	27.813	1.00	22.72
1905	C	SER	A	141	71.707	52.157	26.439	1.00	20.99
1906	O	SER	A	141	72.535	51.344	26.874	1.00	21.12
1907	N	ASP	A	142	70.435	51.840	26.157	1.00	20.94
1909	CA	ASP	A	142	69.803	50.583	26.617	1.00	21.52
1911	CB	ASP	A	142	68.510	50.885	27.360	1.00	21.35
1914	CG	ASP	A	142	68.740	51.573	28.668	1.00	23.16
1915	OD1	ASP	A	142	67.745	52.038	29.261	1.00	22.75
1916	OD2	ASP	A	142	69.871	51.678	29.188	1.00	24.41
1917	C	ASP	A	142	69.436	49.569	25.557	1.00	21.65
1918	O	ASP	A	142	69.308	48.382	25.850	1.00	20.45
1919	N	ALA	A	143	69.203	50.033	24.342	1.00	22.42
1921	CA	ALA	A	143	68.645	49.176	23.301	1.00	23.31
1923	CB	ALA	A	143	68.113	50.004	22.165	1.00	22.74
1927	C	ALA	A	143	69.698	48.200	22.795	1.00	24.09
1928	O	ALA	A	143	70.895	48.453	22.888	1.00	24.03
1929	N	ASP	A	144	69.228	47.087	22.256	1.00	25.84
1931	CA	ASP	A	144	70.096	46.051	21.707	1.00	27.11
1933	CB	ASP	A	144	69.309	44.768	21.402	1.00	27.68
1936	CG	ASP	A	144	68.293	44.426	22.469	1.00	31.56
1937	OD1	ASP	A	144	67.116	44.829	22.309	1.00	38.25
1938	OD2	ASP	A	144	68.558	43.752	23.487	1.00	35.92
1939	C	ASP	A	144	70.716	46.563	20.420	1.00	26.94
1940	O	ASP	A	144	69.995	46.966	19.504	1.00	27.42
1941	N	MET	A	145	72.044	46.586	20.374	1.00	27.00

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1943	CA	MET	A	145	72.794	46.828	19.148	1.00	27.40
1945	CB	MET	A	145	73.297	48.273	19.105	1.00	27.32
1948	CG	MET	A	145	72.199	49.301	19.048	1.00	27.17
1951	SD	MET	A	145	72.806	50.970	18.731	1.00	27.97
1952	CE	MET	A	145	73.747	51.294	20.169	1.00	26.35
1956	C	MET	A	145	73.972	45.850	19.125	1.00	28.08
1957	O	MET	A	145	75.099	46.213	19.487	1.00	27.86
1958	N	PRO	A	146	73.702	44.596	18.768	1.00	28.99
1959	CA	PRO	A	146	74.700	43.519	18.900	1.00	29.80
1961	CB	PRO	A	146	74.018	42.301	18.244	1.00	30.17
1964	CG	PRO	A	146	72.730	42.788	17.654	1.00	29.78
1967	CD	PRO	A	146	72.402	44.090	18.296	1.00	29.22
1970	C	PRO	A	146	76.088	43.778	18.280	1.00	29.90
1971	O	PRO	A	146	77.081	43.394	18.874	1.00	30.77
1972	N	GLU	A	147	76.176	44.452	17.149	1.00	30.07
1974	CA	GLU	A	147	77.488	44.605	16.495	1.00	30.29
1976	CB	GLU	A	147	77.348	44.666	14.970	1.00	30.88
1979	CG	GLU	A	147	76.419	43.625	14.368	1.00	33.60
1982	CD	GLU	A	147	74.996	44.126	14.226	1.00	36.03
1983	OE1	GLU	A	147	74.447	44.088	13.102	1.00	38.00
1984	OE2	GLU	A	147	74.433	44.556	15.252	1.00	37.12
1985	C	GLU	A	147	78.224	45.857	16.976	1.00	28.68
1986	O	GLU	A	147	79.335	46.129	16.528	1.00	28.50
1987	N	VAL	A	148	77.599	46.613	17.879	1.00	26.68
1989	CA	VAL	A	148	78.056	47.949	18.205	1.00	25.01
1991	CB	VAL	A	148	76.886	48.966	18.244	1.00	25.12
1993	CG1	VAL	A	148	77.404	50.369	18.438	1.00	24.25
1997	CG2	VAL	A	148	76.049	48.887	16.950	1.00	24.80
2001	C	VAL	A	148	78.819	47.927	19.526	1.00	23.84
2002	O	VAL	A	148	78.271	47.605	20.585	1.00	23.11
2003	N	SER	A	149	80.098	48.254	19.440	1.00	22.76
2005	CA	SER	A	149	80.952	48.338	20.613	1.00	22.78
2007	CB	SER	A	149	82.404	48.597	20.186	1.00	22.49
2010	OG	SER	A	149	82.568	49.915	19.707	1.00	21.57
2012	C	SER	A	149	80.458	49.448	21.539	1.00	23.11
2013	O	SER	A	149	79.794	50.402	21.099	1.00	21.95
2014	N	ASP	A	150	80.777	49.313	22.817	1.00	23.66
2016	CA	ASP	A	150	80.499	50.348	23.801	1.00	24.49
2018	CB	ASP	A	150	81.010	49.930	25.172	1.00	25.14
2021	CG	ASP	A	150	80.256	48.733	25.735	1.00	27.65
2022	OD1	ASP	A	150	80.719	48.186	26.762	1.00	31.30
2023	OD2	ASP	A	150	79.201	48.281	25.225	1.00	27.89
2024	C	ASP	A	150	81.115	51.680	23.394	1.00	24.45
2025	O	ASP	A	150	80.499	52.725	23.568	1.00	23.41
2026	N	ARG	A	151	82.319	51.639	22.827	1.00	24.28
2028	CA	ARG	A	151	82.973	52.844	22.355	1.00	24.79
2030	CB	ARG	A	151	84.352	52.508	21.759	1.00	26.00
2033	CG	ARG	A	151	85.134	53.699	21.268	1.00	28.93
2036	CD	ARG	A	151	85.432	54.712	22.350	1.00	34.80
2039	NE	ARG	A	151	84.576	55.893	22.233	1.00	38.89
2041	CZ	ARG	A	151	84.277	56.711	23.229	1.00	42.07
2042	NH1	ARG	A	151	83.494	57.756	22.989	1.00	43.97

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2045	NH2	ARG	A	151	84.754	56.502	24.462	1.00	42.69
2048	C	ARG	A	151	82.119	53.534	21.303	1.00	23.63
2049	O	ARG	A	151	81.949	54.749	21.330	1.00	22.68
2050	N	ASP	A	152	81.578	52.751	20.377	1.00	22.64
2052	CA	ASP	A	152	80.765	53.305	19.316	1.00	22.05
2054	CB	ASP	A	152	80.695	52.351	18.126	1.00	22.68
2057	CG	ASP	A	152	82.013	52.303	17.348	1.00	24.58
2058	OD1	ASP	A	152	82.780	53.285	17.412	1.00	24.51
2059	OD2	ASP	A	152	82.369	51.328	16.654	1.00	27.53
2060	C	ASP	A	152	79.380	53.730	19.832	1.00	20.89
2061	O	ASP	A	152	78.829	54.703	19.348	1.00	19.41
2062	N	ARG	A	153	78.855	53.043	20.844	1.00	19.83
2064	CA	ARG	A	153	77.577	53.435	21.459	1.00	18.66
2066	CB	ARG	A	153	77.116	52.390	22.450	1.00	18.96
2069	CG	ARG	A	153	75.734	52.644	23.008	1.00	18.87
2072	CD	ARG	A	153	75.377	51.687	24.112	1.00	19.73
2075	NE	ARG	A	153	75.180	50.322	23.630	1.00	20.07
2077	CZ	ARG	A	153	73.991	49.773	23.369	1.00	22.06
2078	NH1	ARG	A	153	73.929	48.516	22.949	1.00	20.83
2081	NH2	ARG	A	153	72.862	50.466	23.521	1.00	23.23
2084	C	ARG	A	153	77.724	54.771	22.171	1.00	18.18
2085	O	ARG	A	153	76.842	55.612	22.081	1.00	17.20
2086	N	ILE	A	154	78.847	54.959	22.869	1.00	17.73
2088	CA	ILE	A	154	79.141	56.223	23.542	1.00	18.41
2090	CB	ILE	A	154	80.414	56.100	24.449	1.00	18.14
2092	CG1	ILE	A	154	80.092	55.249	25.684	1.00	19.24
2095	CD1	ILE	A	154	81.307	54.703	26.408	1.00	20.01
2099	CG2	ILE	A	154	80.932	57.468	24.875	1.00	19.53
2103	C	ILE	A	154	79.277	57.343	22.505	1.00	17.74
2104	O	ILE	A	154	78.757	58.424	22.698	1.00	18.17
2105	N	SER	A	155	79.934	57.063	21.388	1.00	18.18
2107	CA	SER	A	155	80.095	58.043	20.323	1.00	18.52
2109	CB	SER	A	155	81.020	57.511	19.236	1.00	18.63
2112	OG	SER	A	155	82.330	57.395	19.748	1.00	18.50
2114	C	SER	A	155	78.744	58.437	19.718	1.00	19.05
2115	O	SER	A	155	78.538	59.594	19.368	1.00	19.13
2116	N	MET	A	156	77.836	57.476	19.618	1.00	19.12
2118	CA	MET	A	156	76.482	57.743	19.135	1.00	19.40
2120	CB	MET	A	156	75.674	56.461	19.063	1.00	19.56
2123	CG	MET	A	156	76.083	55.564	17.948	1.00	22.23
2126	SD	MET	A	156	74.922	54.182	17.803	1.00	28.16
2127	CE	MET	A	156	75.814	53.241	16.666	1.00	26.77
2131	C	MET	A	156	75.746	58.693	20.039	1.00	18.61
2132	O	MET	A	156	75.101	59.609	19.567	1.00	18.79
2133	N	ILE	A	157	75.826	58.439	21.342	1.00	18.55
2135	CA	ILE	A	157	75.194	59.281	22.349	1.00	17.91
2137	CB	ILE	A	157	75.342	58.649	23.752	1.00	17.84
2139	CG1	ILE	A	157	74.511	57.360	23.840	1.00	18.27
2142	CD1	ILE	A	157	74.814	56.495	25.017	1.00	18.88
2146	CG2	ILE	A	157	74.941	59.646	24.845	1.00	17.97
2150	C	ILE	A	157	75.804	60.685	22.313	1.00	17.61
2151	O	ILE	A	157	75.087	61.683	22.308	1.00	16.93

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2152	N	SER	A	158	77.136	60.749	22.290	1.00	17.36
2154	CA	SER	A	158	77.856	62.012	22.247	1.00	17.24
2156	CB	SER	A	158	79.372	61.759	22.292	1.00	17.57
2159	OG	SER	A	158	80.087	62.908	21.936	1.00	16.92
2161	C	SER	A	158	77.487	62.819	21.007	1.00	17.58
2162	O	SER	A	158	77.266	64.003	21.093	1.00	17.17
2163	N	GLU	A	159	77.408	62.163	19.856	1.00	18.38
2165	CA	GLU	A	159	77.042	62.833	18.616	1.00	18.63
2167	CB	GLU	A	159	77.242	61.904	17.409	1.00	19.18
2170	CG	GLU	A	159	76.518	62.361	16.145	1.00	20.77
2173	CD	GLU	A	159	76.979	63.726	15.666	1.00	23.75
2174	OE1	GLU	A	159	78.105	64.141	16.022	1.00	24.45
2175	OE2	GLU	A	159	76.233	64.384	14.918	1.00	26.52
2176	C	GLU	A	159	75.592	63.324	18.648	1.00	18.90
2177	O	GLU	A	159	75.311	64.455	18.224	1.00	18.41
2178	N	LEU	A	160	74.671	62.489	19.122	1.00	18.15
2180	CA	LEU	A	160	73.274	62.921	19.169	1.00	18.98
2182	CB	LEU	A	160	72.333	61.801	19.559	1.00	19.20
2185	CG	LEU	A	160	70.845	62.123	19.337	1.00	20.03
2187	CD1	LEU	A	160	70.528	62.479	17.890	1.00	20.04
2191	CD2	LEU	A	160	70.015	60.977	19.795	1.00	21.02
2195	C	LEU	A	160	73.119	64.115	20.113	1.00	19.39
2196	O	LEU	A	160	72.388	65.058	19.808	1.00	19.39
2197	N	ALA	A	161	73.832	64.078	21.234	1.00	19.92
2199	CA	ALA	A	161	73.814	65.162	22.208	1.00	20.54
2201	CB	ALA	A	161	74.591	64.764	23.463	1.00	20.76
2205	C	ALA	A	161	74.362	66.466	21.621	1.00	20.84
2206	O	ALA	A	161	73.690	67.496	21.678	1.00	21.05
2207	N	SER	A	162	75.554	66.431	21.027	1.00	21.51
2209	CA	SER	A	162	76.138	67.660	20.486	1.00	22.08
2211	CB	SER	A	162	77.614	67.492	20.063	1.00	22.37
2214	OG	SER	A	162	77.809	66.365	19.248	1.00	24.18
2216	C	SER	A	162	75.286	68.207	19.336	1.00	21.42
2217	O	SER	A	162	75.142	69.415	19.197	1.00	21.65
2218	N	ALA	A	163	74.700	67.316	18.539	1.00	20.43
2220	CA	ALA	A	163	73.906	67.716	17.379	1.00	20.07
2222	CB	ALA	A	163	73.732	66.523	16.438	1.00	20.07
2226	C	ALA	A	163	72.537	68.265	17.768	1.00	19.77
2227	O	ALA	A	163	71.937	69.041	17.026	1.00	18.96
2228	N	SER	A	164	72.026	67.836	18.922	1.00	19.92
2230	CA	SER	A	164	70.677	68.207	19.366	1.00	19.71
2232	CB	SER	A	164	70.061	67.027	20.112	1.00	20.08
2235	OG	SER	A	164	70.098	65.862	19.285	1.00	21.77
2237	C	SER	A	164	70.655	69.452	20.246	1.00	20.10
2238	O	SER	A	164	69.661	70.210	20.271	1.00	18.98
2239	N	GLY	A	165	71.757	69.676	20.958	1.00	19.76
2241	CA	GLY	A	165	71.846	70.733	21.939	1.00	20.35
2244	C	GLY	A	165	72.244	72.081	21.365	1.00	20.96
2245	O	GLY	A	165	71.982	72.393	20.203	1.00	20.86
2246	N	ILE	A	166	72.900	72.879	22.200	1.00	21.84
2248	CA	ILE	A	166	73.170	74.280	21.914	1.00	22.71
2250	CB	ILE	A	166	73.611	74.975	23.242	1.00	23.10

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2252	CG1	ILE	A	166	73.194	76.437	23.239	1.00	23.87
2255	CD1	ILE	A	166	71.710	76.610	23.444	1.00	23.14
2259	CG2	ILE	A	166	75.109	74.770	23.489	1.00	25.44
2263	C	ILE	A	166	74.197	74.443	20.769	1.00	22.75
2264	O	ILE	A	166	74.206	75.456	20.057	1.00	23.12
2265	N	ALA	A	167	75.027	73.422	20.572	1.00	22.36
2267	CA	ALA	A	167	75.954	73.367	19.451	1.00	22.62
2269	CB	ALA	A	167	77.109	72.455	19.770	1.00	22.85
2273	C	ALA	A	167	75.285	72.916	18.152	1.00	22.34
2274	O	ALA	A	167	75.905	72.963	17.111	1.00	22.65
2275	N	GLY	A	168	74.028	72.488	18.212	1.00	21.57
2277	CA	GLY	A	168	73.304	72.064	17.022	1.00	21.12
2280	C	GLY	A	168	71.883	72.588	16.982	1.00	20.68
2281	O	GLY	A	168	71.665	73.785	16.956	1.00	19.79
2282	N	MET	A	169	70.914	71.682	17.005	1.00	20.95
2284	CA	MET	A	169	69.501	72.019	16.812	1.00	20.87
2286	CB	MET	A	169	68.655	70.757	16.927	1.00	21.21
2289	CG	MET	A	169	67.183	70.922	16.531	1.00	22.91
2292	SD	MET	A	169	66.208	71.479	17.897	1.00	28.34
2293	CE	MET	A	169	66.254	69.967	19.003	1.00	25.97
2297	C	MET	A	169	68.952	73.140	17.721	1.00	20.52
2298	O	MET	A	169	68.310	74.072	17.224	1.00	19.77
2299	N	CYS	A	170	69.200	73.059	19.028	1.00	20.60
2301	CA	CYS	A	170	68.689	74.061	19.977	1.00	20.42
2303	CB	BCYS	A	170	68.958	73.590	21.405	0.35	20.62
2304	CB	ACYS	A	170	68.958	73.668	21.427	0.65	20.89
2309	SG	BCYS	A	170	67.803	74.234	22.609	0.35	20.91
2310	SG	ACYS	A	170	67.804	72.489	22.098	0.65	22.71
2311	C	CYS	A	170	69.332	75.426	19.744	1.00	20.33
2312	O	CYS	A	170	68.665	76.459	19.811	1.00	18.74
2313	N	GLY	A	171	70.650	75.414	19.539	1.00	20.11
2315	CA	GLY	A	171	71.384	76.605	19.172	1.00	20.26
2318	C	GLY	A	171	70.807	77.252	17.932	1.00	20.35
2319	O	GLY	A	171	70.645	78.473	17.877	1.00	19.82
2320	N	GLY	A	172	70.470	76.425	16.948	1.00	20.20
2322	CA	GLY	A	172	69.875	76.891	15.715	1.00	20.43
2325	C	GLY	A	172	68.484	77.441	15.920	1.00	20.51
2326	O	GLY	A	172	68.117	78.435	15.303	1.00	20.93
2327	N	GLN	A	173	67.716	76.816	16.800	1.00	20.70
2329	CA	GLN	A	173	66.397	77.327	17.168	1.00	21.15
2331	CB	GLN	A	173	65.684	76.383	18.149	1.00	21.47
2334	CG	GLN	A	173	65.165	75.072	17.546	1.00	21.62
2337	CD	GLN	A	173	64.102	75.279	16.494	1.00	22.97
2338	OE1	GLN	A	173	64.417	75.656	15.362	1.00	27.11
2339	NE2	GLN	A	173	62.845	75.031	16.850	1.00	22.24
2342	C	GLN	A	173	66.514	78.725	17.794	1.00	21.59
2343	O	GLN	A	173	65.695	79.609	17.513	1.00	22.14
2344	N	ALA	A	174	67.532	78.931	18.622	1.00	21.59
2346	CA	ALA	A	174	67.766	80.245	19.230	1.00	21.99
2348	CB	ALA	A	174	68.847	80.166	20.296	1.00	22.20
2352	C	ALA	A	174	68.152	81.269	18.164	1.00	22.07
2353	O	ALA	A	174	67.683	82.380	18.206	1.00	21.87

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2354	N	LEU	A	175	69.001	80.885	17.212	1.00	22.13
2356	CA	LEU	A	175	69.369	81.776	16.106	1.00	23.00
2358	CB	LEU	A	175	70.449	81.144	15.233	1.00	23.09
2361	CG	LEU	A	175	71.824	80.871	15.840	1.00	22.66
2363	CD1	LEU	A	175	72.668	80.085	14.817	1.00	24.29
2367	CD2	LEU	A	175	72.522	82.155	16.235	1.00	22.45
2371	C	LEU	A	175	68.163	82.119	15.240	1.00	23.28
2372	O	LEU	A	175	68.003	83.265	14.805	1.00	23.62
2373	N	ASP	A	176	67.314	81.123	15.002	1.00	23.53
2375	CA	ASP	A	176	66.112	81.280	14.197	1.00	24.49
2377	CB	ASP	A	176	65.382	79.934	14.080	1.00	24.90
2380	CG	ASP	A	176	64.004	80.064	13.491	1.00	25.57
2381	OD1	ASP	A	176	63.830	79.750	12.287	1.00	28.64
2382	OD2	ASP	A	176	63.023	80.441	14.162	1.00	28.54
2383	C	ASP	A	176	65.187	82.320	14.841	1.00	24.97
2384	O	ASP	A	176	64.683	83.222	14.178	1.00	24.47
2385	N	LEU	A	177	64.974	82.168	16.138	1.00	25.23
2387	CA	LEU	A	177	64.127	83.083	16.905	1.00	26.68
2389	CB	LEU	A	177	63.977	82.575	18.343	1.00	26.78
2392	CG	LEU	A	177	62.658	81.902	18.734	1.00	28.22
2394	CD1	LEU	A	177	62.016	81.077	17.633	1.00	29.14
2398	CD2	LEU	A	177	62.892	81.055	19.970	1.00	29.13
2402	C	LEU	A	177	64.686	84.512	16.914	1.00	26.76
2403	O	LEU	A	177	63.936	85.474	16.784	1.00	26.89
2404	N	ASP	A	178	66.002	84.640	17.050	1.00	27.40
2406	CA	ASP	A	178	66.636	85.952	17.078	1.00	28.30
2408	CB	ASP	A	178	68.107	85.827	17.459	1.00	28.53
2411	CG	ASP	A	178	68.753	87.176	17.720	1.00	31.35
2412	OD1	ASP	A	178	69.682	87.571	16.965	1.00	33.39
2413	OD2	ASP	A	178	68.389	87.907	18.667	1.00	33.95
2414	C	ASP	A	178	66.513	86.681	15.734	1.00	28.03
2415	O	ASP	A	178	66.398	87.907	15.689	1.00	27.69
2416	N	ALA	A	179	66.525	85.915	14.648	1.00	27.46
2418	CA	ALA	A	179	66.499	86.467	13.300	1.00	27.69
2420	CB	ALA	A	179	67.174	85.479	12.330	1.00	27.70
2424	C	ALA	A	179	65.089	86.843	12.796	1.00	27.58
2425	O	ALA	A	179	64.946	87.351	11.683	1.00	27.80
2426	N	GLU	A	180	64.057	86.590	13.596	1.00	27.88
2428	CA	GLU	A	180	62.702	87.040	13.277	1.00	28.36
2430	CB	GLU	A	180	61.710	86.633	14.367	1.00	28.57
2433	CG	GLU	A	180	61.415	85.151	14.422	1.00	29.97
2436	CD	GLU	A	180	60.434	84.780	15.517	1.00	32.47
2437	OE1	GLU	A	180	60.070	85.661	16.338	1.00	34.93
2438	OE2	GLU	A	180	60.026	83.598	15.558	1.00	32.41
2439	C	GLU	A	180	62.695	88.560	13.162	1.00	28.40
2440	O	GLU	A	180	63.140	89.252	14.075	1.00	27.70
2441	N	GLY	A	181	62.227	89.057	12.020	1.00	28.55
2443	CA	GLY	A	181	62.105	90.477	11.766	1.00	29.05
2446	C	GLY	A	181	63.391	91.173	11.391	1.00	29.41
2447	O	GLY	A	181	63.379	92.382	11.129	1.00	30.34
2448	N	LYS	A	182	64.501	90.437	11.353	1.00	29.52
2450	CA	LYS	A	182	65.818	91.032	11.137	1.00	29.58

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2452	CB	LYS	A	182	66.807	90.510	12.175	1.00	30.25
2455	CG	LYS	A	182	66.415	90.819	13.604	1.00	31.19
2458	CD	LYS	A	182	67.528	90.474	14.569	1.00	33.42
2461	CE	LYS	A	182	67.168	90.894	16.009	1.00	34.43
2464	NZ	LYS	A	182	65.969	90.178	16.544	1.00	36.01
2468	C	LYS	A	182	66.375	90.797	9.730	1.00	29.61
2469	O	LYS	A	182	67.389	91.383	9.367	1.00	29.31
2470	N	HIS	A	183	65.725	89.944	8.947	1.00	29.18
2472	CA	HIS	A	183	66.098	89.736	7.546	1.00	29.54
2474	CB	HIS	A	183	65.574	90.895	6.688	1.00	29.50
2477	CG	HIS	A	183	64.099	91.086	6.806	1.00	29.04
2478	ND1	HIS	A	183	63.217	90.679	5.835	1.00	29.33
2480	CE1	HIS	A	183	61.982	90.944	6.226	1.00	30.87
2482	NE2	HIS	A	183	62.033	91.486	7.429	1.00	30.77
2484	CD2	HIS	A	183	63.346	91.580	7.816	1.00	30.69
2486	C	HIS	A	183	67.598	89.588	7.410	1.00	29.56
2487	O	HIS	A	183	68.261	90.375	6.732	1.00	29.82
2488	N	VAL	A	184	68.136	88.569	8.067	1.00	29.52
2490	CA	VAL	A	184	69.580	88.461	8.215	1.00	29.40
2492	CB	VAL	A	184	69.976	87.488	9.352	1.00	29.29
2494	CG1	VAL	A	184	69.310	87.904	10.659	1.00	29.32
2498	CG2	VAL	A	184	69.645	86.033	8.998	1.00	28.66
2502	C	VAL	A	184	70.233	88.072	6.886	1.00	29.41
2503	O	VAL	A	184	69.586	87.448	6.037	1.00	29.64
2504	N	PRO	A	185	71.501	88.441	6.701	1.00	29.70
2505	CA	PRO	A	185	72.217	88.146	5.458	1.00	29.74
2507	CB	PRO	A	185	73.565	88.851	5.643	1.00	29.72
2510	CG	PRO	A	185	73.389	89.766	6.777	1.00	30.18
2513	CD	PRO	A	185	72.357	89.168	7.653	1.00	30.09
2516	C	PRO	A	185	72.448	86.659	5.266	1.00	29.95
2517	O	PRO	A	185	72.317	85.896	6.224	1.00	29.23
2518	N	LEU	A	186	72.843	86.279	4.059	1.00	30.11
2520	CA	LEU	A	186	73.010	84.873	3.690	1.00	30.66
2522	CB	LEU	A	186	73.595	84.765	2.281	1.00	30.90
2525	CG	LEU	A	186	73.604	83.417	1.548	1.00	32.07
2527	CD1	LEU	A	186	74.931	82.695	1.750	1.00	34.56
2531	CD2	LEU	A	186	72.438	82.535	1.942	1.00	31.83
2535	C	LEU	A	186	73.875	84.071	4.670	1.00	30.74
2536	O	LEU	A	186	73.472	82.997	5.093	1.00	30.04
2537	N	ASP	A	187	75.058	84.584	5.009	1.00	30.98
2539	CA	ASP	A	187	75.951	83.903	5.945	1.00	31.77
2541	CB	ASP	A	187	77.278	84.667	6.143	1.00	32.58
2544	CG	ASP	A	187	77.097	86.128	6.641	1.00	34.74
2545	OD1	ASP	A	187	75.963	86.630	6.812	1.00	37.70
2546	OD2	ASP	A	187	78.079	86.866	6.881	1.00	39.45
2547	C	ASP	A	187	75.295	83.578	7.301	1.00	31.43
2548	O	ASP	A	187	75.516	82.494	7.847	1.00	31.36
2549	N	ALA	A	188	74.493	84.505	7.823	1.00	30.71
2551	CA	ALA	A	188	73.781	84.297	9.082	1.00	30.32
2553	CB	ALA	A	188	73.271	85.624	9.641	1.00	30.46
2557	C	ALA	A	188	72.627	83.331	8.870	1.00	29.80
2558	O	ALA	A	188	72.328	82.505	9.731	1.00	28.47

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2559	N	LEU	A	189	71.990	83.427	7.708	1.00	29.23
2561	CA	LEU	A	189	70.902	82.529	7.358	1.00	29.70
2563	CB	LEU	A	189	70.360	82.867	5.971	1.00	30.15
2566	CG	LEU	A	189	68.870	83.128	5.772	1.00	31.79
2568	CD1	LEU	A	189	68.545	82.912	4.280	1.00	32.57
2572	CD2	LEU	A	189	67.958	82.296	6.672	1.00	32.39
2576	C	LEU	A	189	71.397	81.077	7.356	1.00	29.25
2577	O	LEU	A	189	70.766	80.182	7.923	1.00	27.68
2578	N	GLU	A	190	72.539	80.867	6.712	1.00	28.91
2580	CA	GLU	A	190	73.138	79.547	6.604	1.00	28.82
2582	CB	GLU	A	190	74.362	79.609	5.697	1.00	29.44
2585	CG	GLU	A	190	74.926	78.249	5.322	1.00	31.65
2588	CD	GLU	A	190	76.119	78.345	4.382	1.00	35.05
2589	OE1	GLU	A	190	76.048	79.127	3.405	1.00	36.65
2590	OE2	GLU	A	190	77.126	77.631	4.625	1.00	37.41
2591	C	GLU	A	190	73.524	78.996	7.972	1.00	28.22
2592	O	GLU	A	190	73.406	77.807	8.220	1.00	27.03
2593	N	ARG	A	191	74.001	79.866	8.856	1.00	27.79
2595	CA	ARG	A	191	74.342	79.454	10.210	1.00	27.69
2597	CB	ARG	A	191	75.021	80.585	10.988	1.00	28.29
2600	CG	ARG	A	191	76.429	80.908	10.483	1.00	32.30
2603	CD	ARG	A	191	77.323	81.682	11.474	1.00	35.96
2606	NE	ARG	A	191	78.509	80.902	11.831	1.00	39.49
2608	CZ	ARG	A	191	79.520	80.619	11.005	1.00	42.00
2609	NH1	ARG	A	191	79.524	81.054	9.748	1.00	43.12
2612	NH2	ARG	A	191	80.539	79.889	11.440	1.00	42.49
2615	C	ARG	A	191	73.100	78.970	10.948	1.00	26.20
2616	O	ARG	A	191	73.153	77.952	11.634	1.00	25.47
2617	N	ILE	A	192	71.985	79.681	10.787	1.00	25.12
2619	CA	ILE	A	192	70.719	79.254	11.387	1.00	24.45
2621	CB	ILE	A	192	69.546	80.183	11.009	1.00	24.28
2623	CG1	ILE	A	192	69.717	81.579	11.619	1.00	25.03
2626	CD1	ILE	A	192	68.851	82.624	10.981	1.00	25.02
2630	CG2	ILE	A	192	68.222	79.577	11.474	1.00	24.54
2634	C	ILE	A	192	70.385	77.842	10.906	1.00	24.27
2635	O	ILE	A	192	70.205	76.928	11.699	1.00	23.05
2636	N	HIS	A	193	70.289	77.701	9.590	1.00	23.44
2638	CA	HIS	A	193	69.789	76.477	8.976	1.00	23.31
2640	CB	HIS	A	193	69.573	76.731	7.485	1.00	23.43
2643	CG	HIS	A	193	68.349	77.547	7.209	1.00	24.48
2644	ND1	HIS	A	193	67.494	77.964	8.208	1.00	25.73
2646	CE1	HIS	A	193	66.480	78.623	7.675	1.00	26.42
2648	NE2	HIS	A	193	66.659	78.669	6.367	1.00	25.37
2650	CD2	HIS	A	193	67.817	77.999	6.052	1.00	25.77
2652	C	HIS	A	193	70.678	75.264	9.230	1.00	22.37
2653	O	HIS	A	193	70.179	74.181	9.534	1.00	22.47
2654	N	ARG	A	194	71.986	75.445	9.128	1.00	21.53
2656	CA	ARG	A	194	72.919	74.362	9.391	1.00	21.47
2658	CB	ARG	A	194	74.358	74.778	9.120	1.00	20.83
2661	CG	ARG	A	194	74.700	74.835	7.656	1.00	21.22
2664	CD	ARG	A	194	76.180	74.847	7.423	1.00	22.88
2667	NE	ARG	A	194	76.501	75.077	6.022	1.00	24.27

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2669	CZ	ARG	A	194	76.459	74.147	5.092	1.00	25.12
2670	NH1	ARG	A	194	76.120	72.904	5.398	1.00	25.42
2673	NH2	ARG	A	194	76.784	74.455	3.840	1.00	28.83
2676	C	ARG	A	194	72.780	73.872	10.829	1.00	21.18
2677	O	ARG	A	194	72.861	72.681	11.071	1.00	20.79
2678	N	HIS	A	195	72.583	74.777	11.784	1.00	21.00
2680	CA	HIS	A	195	72.436	74.337	13.171	1.00	21.63
2682	CB	HIS	A	195	72.773	75.458	14.158	1.00	21.62
2685	CG	HIS	A	195	74.232	75.787	14.215	1.00	24.46
2686	ND1	HIS	A	195	74.944	75.833	15.394	1.00	28.06
2688	CE1	HIS	A	195	76.201	76.148	15.134	1.00	28.87
2690	NE2	HIS	A	195	76.330	76.304	13.831	1.00	29.50
2692	CD2	HIS	A	195	75.113	76.086	13.233	1.00	27.40
2694	C	HIS	A	195	71.050	73.751	13.451	1.00	21.00
2695	O	HIS	A	195	70.948	72.646	13.985	1.00	20.86
2696	N	LYS	A	196	69.985	74.462	13.087	1.00	20.63
2698	CA	LYS	A	196	68.642	74.022	13.489	1.00	20.10
2700	CB	LYS	A	196	67.590	75.123	13.367	1.00	19.88
2703	CG	LYS	A	196	66.987	75.363	11.997	1.00	19.59
2706	CD	LYS	A	196	65.944	76.473	12.065	1.00	19.02
2709	CE	LYS	A	196	65.416	76.847	10.672	1.00	18.63
2712	NZ	LYS	A	196	64.064	77.494	10.673	1.00	19.09
2716	C	LYS	A	196	68.215	72.756	12.758	1.00	20.00
2717	O	LYS	A	196	67.491	71.960	13.307	1.00	20.23
2718	N	THR	A	197	68.705	72.557	11.539	1.00	19.63
2720	CA	THR	A	197	68.278	71.433	10.726	1.00	19.13
2722	CB	THR	A	197	67.408	71.938	9.580	1.00	19.35
2724	OG1	THR	A	197	66.166	72.400	10.127	1.00	18.33
2726	CG2	THR	A	197	67.021	70.812	8.618	1.00	18.67
2730	C	THR	A	197	69.413	70.554	10.226	1.00	19.03
2731	O	THR	A	197	69.275	69.332	10.223	1.00	18.17
2732	N	GLY	A	198	70.522	71.167	9.812	1.00	19.30
2734	CA	GLY	A	198	71.667	70.421	9.316	1.00	19.16
2737	C	GLY	A	198	72.260	69.466	10.329	1.00	19.28
2738	O	GLY	A	198	72.580	68.330	9.987	1.00	19.12
2739	N	ALA	A	199	72.371	69.910	11.576	1.00	19.18
2741	CA	ALA	A	199	73.129	69.182	12.585	1.00	19.36
2743	CB	ALA	A	199	73.245	70.005	13.861	1.00	19.70
2747	C	ALA	A	199	72.505	67.816	12.897	1.00	19.34
2748	O	ALA	A	199	73.224	66.830	13.057	1.00	19.28
2749	N	LEU	A	200	71.177	67.768	12.994	1.00	19.51
2751	CA	LEU	A	200	70.476	66.522	13.302	1.00	19.63
2753	CB	LEU	A	200	69.016	66.775	13.700	1.00	19.77
2756	CG	LEU	A	200	68.261	65.516	14.183	1.00	20.34
2758	CD1	LEU	A	200	68.918	64.931	15.431	1.00	20.63
2762	CD2	LEU	A	200	66.799	65.855	14.449	1.00	20.55
2766	C	LEU	A	200	70.514	65.563	12.125	1.00	19.55
2767	O	LEU	A	200	70.590	64.336	12.312	1.00	19.72
2768	N	ILE	A	201	70.462	66.114	10.919	1.00	19.19
2770	CA	ILE	A	201	70.556	65.299	9.706	1.00	19.51
2772	CB	ILE	A	201	70.178	66.143	8.471	1.00	19.64
2774	CG1	ILE	A	201	68.659	66.197	8.372	1.00	20.21

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2777	CD1	ILE	A	201	68.149	67.249	7.449	1.00	21.65
2781	CG2	ILE	A	201	70.782	65.578	7.169	1.00	20.92
2785	C	ILE	A	201	71.941	64.661	9.604	1.00	19.17
2786	O	ILE	A	201	72.066	63.504	9.227	1.00	18.77
2787	N	ARG	A	202	72.970	65.420	9.963	1.00	19.39
2789	CA	ARG	A	202	74.323	64.891	10.001	1.00	19.72
2791	CB	ARG	A	202	75.343	66.008	10.148	1.00	20.03
2794	CG	ARG	A	202	76.774	65.526	10.119	1.00	21.06
2797	CD	ARG	A	202	77.777	66.638	10.165	1.00	20.98
2800	NE	ARG	A	202	77.824	67.265	11.473	1.00	23.53
2802	CZ	ARG	A	202	78.617	68.294	11.789	1.00	25.30
2803	NH1	ARG	A	202	78.580	68.800	13.012	1.00	23.66
2806	NH2	ARG	A	202	79.445	68.815	10.891	1.00	26.69
2809	C	ARG	A	202	74.453	63.843	11.113	1.00	19.73
2810	O	ARG	A	202	75.153	62.859	10.935	1.00	19.84
2811	N	ALA	A	203	73.741	64.027	12.226	1.00	19.24
2813	CA	ALA	A	203	73.713	63.009	13.276	1.00	18.65
2815	CB	ALA	A	203	73.001	63.513	14.517	1.00	19.04
2819	C	ALA	A	203	73.097	61.696	12.824	1.00	18.20
2820	O	ALA	A	203	73.582	60.644	13.210	1.00	18.83
2821	N	ALA	A	204	72.025	61.740	12.043	1.00	18.01
2823	CA	ALA	A	204	71.441	60.524	11.485	1.00	18.08
2825	CB	ALA	A	204	70.268	60.868	10.588	1.00	18.17
2829	C	ALA	A	204	72.481	59.738	10.700	1.00	18.04
2830	O	ALA	A	204	72.645	58.522	10.879	1.00	17.73
2831	N	VAL	A	205	73.170	60.430	9.809	1.00	17.87
2833	CA	VAL	A	205	74.174	59.786	8.990	1.00	18.48
2835	CB	VAL	A	205	74.659	60.714	7.874	1.00	18.22
2837	CG1	VAL	A	205	75.791	60.079	7.109	1.00	18.92
2841	CG2	VAL	A	205	73.476	61.057	6.930	1.00	17.58
2845	C	VAL	A	205	75.314	59.238	9.852	1.00	18.69
2846	O	VAL	A	205	75.716	58.086	9.677	1.00	20.23
2847	N	ARG	A	206	75.783	60.032	10.808	1.00	18.74
2849	CA	ARG	A	206	76.862	59.629	11.702	1.00	18.96
2851	CB	ARG	A	206	77.274	60.778	12.615	1.00	18.76
2854	CG	ARG	A	206	78.157	61.792	11.948	1.00	19.71
2857	CD	ARG	A	206	78.477	63.008	12.803	1.00	19.66
2860	NE	ARG	A	206	79.481	63.857	12.167	1.00	21.03
2862	CZ	ARG	A	206	80.008	64.936	12.737	1.00	22.60
2863	NH1	ARG	A	206	79.659	65.289	13.965	1.00	22.08
2866	NH2	ARG	A	206	80.903	65.660	12.079	1.00	21.63
2869	C	ARG	A	206	76.481	58.427	12.549	1.00	19.18
2870	O	ARG	A	206	77.283	57.530	12.757	1.00	18.61
2871	N	LEU	A	207	75.244	58.394	13.014	1.00	19.73
2873	CA	LEU	A	207	74.790	57.288	13.850	1.00	20.29
2875	CB	LEU	A	207	73.426	57.600	14.481	1.00	20.21
2878	CG	LEU	A	207	73.432	58.067	15.944	1.00	21.69
2880	CD1	LEU	A	207	74.453	59.147	16.210	1.00	22.70
2884	CD2	LEU	A	207	72.044	58.554	16.298	1.00	23.52
2888	C	LEU	A	207	74.715	56.013	13.013	1.00	20.31
2889	O	LEU	A	207	75.049	54.941	13.486	1.00	19.90
2890	N	GLY	A	208	74.273	56.131	11.772	1.00	20.46

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2892	CA	GLY	A	208	74.297	55.000	10.861	1.00	21.15
2895	C	GLY	A	208	75.703	54.457	10.656	1.00	21.20
2896	O	GLY	A	208	75.933	53.240	10.737	1.00	22.15
2897	N	ALA	A	209	76.643	55.362	10.419	1.00	21.27
2899	CA	ALA	A	209	78.046	55.006	10.215	1.00	22.05
2901	CB	ALA	A	209	78.813	56.193	9.733	1.00	21.96
2905	C	ALA	A	209	78.700	54.419	11.480	1.00	22.41
2906	O	ALA	A	209	79.383	53.398	11.411	1.00	22.53
2907	N	LEU	A	210	78.471	55.041	12.635	1.00	22.29
2909	CA	LEU	A	210	79.090	54.580	13.877	1.00	22.51
2911	CB	LEU	A	210	78.775	55.522	15.039	1.00	22.37
2914	CG	LEU	A	210	79.513	56.853	14.977	1.00	22.40
2916	CD1	LEU	A	210	78.845	57.900	15.863	1.00	22.42
2920	CD2	LEU	A	210	81.004	56.689	15.372	1.00	22.32
2924	C	LEU	A	210	78.642	53.168	14.213	1.00	23.22
2925	O	LEU	A	210	79.383	52.408	14.830	1.00	23.30
2926	N	SER	A	211	77.430	52.809	13.786	1.00	24.01
2928	CA	SER	A	211	76.914	51.469	13.999	1.00	24.10
2930	CB	SER	A	211	75.478	51.347	13.496	1.00	24.10
2933	OG	SER	A	211	75.459	51.162	12.104	1.00	25.59
2935	C	SER	A	211	77.764	50.397	13.335	1.00	24.24
2936	O	SER	A	211	77.746	49.254	13.778	1.00	23.60
2937	N	ALA	A	212	78.464	50.782	12.269	1.00	24.79
2939	CA	ALA	A	212	79.332	49.906	11.496	1.00	25.88
2941	CB	ALA	A	212	79.361	50.376	10.050	1.00	26.06
2945	C	ALA	A	212	80.762	49.837	12.044	1.00	26.25
2946	O	ALA	A	212	81.602	49.130	11.490	1.00	27.04
2947	N	GLY	A	213	81.051	50.586	13.100	1.00	26.38
2949	CA	GLY	A	213	82.373	50.574	13.692	1.00	27.08
2952	C	GLY	A	213	83.427	51.209	12.809	1.00	27.54
2953	O	GLY	A	213	83.193	52.242	12.199	1.00	27.58
2954	N	ASP	A	214	84.584	50.570	12.718	1.00	28.92
2956	CA	ASP	A	214	85.758	51.188	12.105	1.00	29.67
2958	CB	ASP	A	214	86.993	50.294	12.281	1.00	30.31
2961	CG	ASP	A	214	87.596	50.413	13.666	1.00	33.03
2962	OD1	ASP	A	214	88.445	49.568	14.020	1.00	37.45
2963	OD2	ASP	A	214	87.285	51.318	14.478	1.00	35.85
2964	C	ASP	A	214	85.530	51.523	10.650	1.00	29.40
2965	O	ASP	A	214	85.907	52.596	10.203	1.00	29.23
2966	N	LYS	A	215	84.879	50.625	9.921	1.00	29.50
2968	CA	LYS	A	215	84.593	50.862	8.505	1.00	29.92
2970	CB	LYS	A	215	84.019	49.610	7.839	1.00	30.45
2973	CG	LYS	A	215	85.103	48.766	7.182	1.00	33.43
2976	CD	LYS	A	215	84.685	47.310	6.964	1.00	36.17
2979	CE	LYS	A	215	85.888	46.439	6.568	1.00	37.55
2982	NZ	LYS	A	215	85.967	45.213	7.416	1.00	39.13
2986	C	LYS	A	215	83.672	52.076	8.312	1.00	29.02
2987	O	LYS	A	215	83.851	52.860	7.384	1.00	27.84
2988	N	GLY	A	216	82.696	52.241	9.198	1.00	28.66
2990	CA	GLY	A	216	81.855	53.429	9.162	1.00	28.17
2993	C	GLY	A	216	82.647	54.692	9.471	1.00	27.77
2994	O	GLY	A	216	82.503	55.719	8.812	1.00	27.08

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2995	N	ARG	A	217	83.498	54.609	10.482	1.00	27.98
2997	CA	ARG	A	217	84.306	55.751	10.900	1.00	28.29
2999	CB	ARG	A	217	85.165	55.391	12.106	1.00	28.55
3002	CG	ARG	A	217	84.449	55.520	13.428	1.00	28.34
3005	CD	ARG	A	217	85.328	55.173	14.580	1.00	29.33
3008	NE	ARG	A	217	84.577	55.110	15.826	1.00	29.90
3010	CZ	ARG	A	217	84.375	56.148	16.637	1.00	29.01
3011	NH1	ARG	A	217	84.836	57.359	16.334	1.00	29.10
3014	NH2	ARG	A	217	83.671	55.980	17.743	1.00	28.00
3017	C	ARG	A	217	85.201	56.266	9.783	1.00	28.80
3018	O	ARG	A	217	85.367	57.476	9.645	1.00	28.97
3019	N	ARG	A	218	85.752	55.354	8.978	1.00	29.00
3021	CA	ARG	A	218	86.622	55.726	7.853	1.00	29.76
3023	CB	ARG	A	218	87.268	54.483	7.223	1.00	30.54
3026	CG	ARG	A	218	88.351	53.812	8.069	1.00	33.89
3029	CD	ARG	A	218	88.273	52.280	8.115	1.00	38.26
3032	NE	ARG	A	218	88.914	51.617	6.975	1.00	41.13
3034	CZ	ARG	A	218	88.318	51.290	5.817	1.00	44.61
3035	NH1	ARG	A	218	89.023	50.681	4.862	1.00	46.06
3038	NH2	ARG	A	218	87.037	51.564	5.587	1.00	45.97
3041	C	ARG	A	218	85.866	56.481	6.765	1.00	29.10
3042	O	ARG	A	218	86.460	57.283	6.034	1.00	29.09
3043	N	ALA	A	219	84.565	56.209	6.646	1.00	27.99
3045	CA	ALA	A	219	83.720	56.894	5.669	1.00	27.60
3047	CB	ALA	A	219	82.532	56.030	5.313	1.00	27.48
3051	C	ALA	A	219	83.234	58.253	6.142	1.00	27.24
3052	O	ALA	A	219	82.710	59.018	5.344	1.00	26.75
3053	N	LEU	A	220	83.394	58.543	7.433	1.00	27.30
3055	CA	LEU	A	220	82.807	59.736	8.036	1.00	27.51
3057	CB	LEU	A	220	83.061	59.804	9.546	1.00	27.81
3060	CG	LEU	A	220	82.127	58.960	10.416	1.00	29.69
3062	CD1	LEU	A	220	82.573	59.004	11.889	1.00	30.50
3066	CD2	LEU	A	220	80.677	59.411	10.271	1.00	30.60
3070	C	LEU	A	220	83.226	61.045	7.400	1.00	26.87
3071	O	LEU	A	220	82.380	61.901	7.232	1.00	27.16
3072	N	PRO	A	221	84.502	61.248	7.067	1.00	26.59
3073	CA	PRO	A	221	84.879	62.502	6.399	1.00	26.30
3075	CB	PRO	A	221	86.349	62.269	6.006	1.00	26.54
3078	CG	PRO	A	221	86.853	61.366	7.081	1.00	27.08
3081	CD	PRO	A	221	85.685	60.415	7.352	1.00	26.58
3084	C	PRO	A	221	83.996	62.758	5.195	1.00	25.66
3085	O	PRO	A	221	83.479	63.859	5.044	1.00	26.22
3086	N	VAL	A	222	83.770	61.735	4.381	1.00	24.71
3088	CA	VAL	A	222	82.965	61.910	3.181	1.00	24.34
3090	CB	VAL	A	222	83.272	60.835	2.139	1.00	24.09
3092	CG1	VAL	A	222	82.302	60.927	0.999	1.00	23.94
3096	CG2	VAL	A	222	84.718	60.988	1.655	1.00	25.44
3100	C	VAL	A	222	81.465	61.955	3.470	1.00	23.78
3101	O	VAL	A	222	80.754	62.771	2.885	1.00	23.40
3102	N	LEU	A	223	80.978	61.096	4.362	1.00	23.25
3104	CA	LEU	A	223	79.552	61.118	4.707	1.00	22.90
3106	CB	LEU	A	223	79.179	59.955	5.627	1.00	23.13

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3109	CG	LEU	A	223	79.130	58.583	4.947	1.00	22.78
3111	CD1	LEU	A	223	79.022	57.462	5.987	1.00	23.57
3115	CD2	LEU	A	223	77.991	58.484	3.975	1.00	23.72
3119	C	LEU	A	223	79.159	62.441	5.346	1.00	23.02
3120	O	LEU	A	223	78.023	62.903	5.182	1.00	22.74
3121	N	ASP	A	224	80.081	63.036	6.093	1.00	23.24
3123	CA	ASP	A	224	79.838	64.328	6.722	1.00	23.61
3125	CB	ASP	A	224	81.028	64.753	7.588	1.00	23.94
3128	CG	ASP	A	224	81.009	64.118	8.974	1.00	25.27
3129	OD1	ASP	A	224	79.961	63.561	9.379	1.00	25.31
3130	OD2	ASP	A	224	81.989	64.158	9.749	1.00	27.02
3131	C	ASP	A	224	79.568	65.385	5.654	1.00	23.60
3132	O	ASP	A	224	78.630	66.175	5.772	1.00	22.89
3133	N	LYS	A	225	80.373	65.377	4.599	1.00	23.58
3135	CA	LYS	A	225	80.234	66.391	3.557	1.00	24.32
3137	CB	LYS	A	225	81.439	66.381	2.594	1.00	24.94
3140	CG	LYS	A	225	82.825	66.478	3.298	1.00	27.64
3143	CD	LYS	A	225	83.113	67.828	4.009	1.00	31.84
3146	CE	LYS	A	225	83.516	67.719	5.546	1.00	32.28
3149	NZ	LYS	A	225	84.063	66.374	6.064	1.00	30.63
3153	C	LYS	A	225	78.901	66.207	2.842	1.00	23.43
3154	O	LYS	A	225	78.205	67.177	2.548	1.00	23.79
3155	N	TYR	A	226	78.521	64.955	2.612	1.00	22.64
3157	CA	TYR	A	226	77.214	64.632	2.063	1.00	21.59
3159	CB	TYR	A	226	77.075	63.114	1.881	1.00	21.93
3162	CG	TYR	A	226	75.645	62.633	1.753	1.00	20.62
3163	CD1	TYR	A	226	75.021	62.606	0.523	1.00	21.37
3165	CE1	TYR	A	226	73.736	62.160	0.386	1.00	20.90
3167	CZ	TYR	A	226	73.030	61.727	1.487	1.00	20.66
3168	OH	TYR	A	226	71.737	61.289	1.311	1.00	21.67
3170	CE2	TYR	A	226	73.617	61.727	2.730	1.00	21.12
3172	CD2	TYR	A	226	74.933	62.174	2.862	1.00	20.69
3174	C	TYR	A	226	76.098	65.121	2.979	1.00	21.19
3175	O	TYR	A	226	75.156	65.754	2.523	1.00	21.30
3176	N	ALA	A	227	76.208	64.804	4.261	1.00	20.68
3178	CA	ALA	A	227	75.173	65.126	5.240	1.00	20.41
3180	CB	ALA	A	227	75.503	64.513	6.581	1.00	20.07
3184	C	ALA	A	227	75.007	66.627	5.390	1.00	20.36
3185	O	ALA	A	227	73.893	67.123	5.485	1.00	19.95
3186	N	GLU	A	228	76.132	67.326	5.407	1.00	20.85
3188	CA	GLU	A	228	76.160	68.786	5.503	1.00	21.65
3190	CB	GLU	A	228	77.601	69.285	5.581	1.00	21.59
3193	CG	GLU	A	228	78.225	69.020	6.940	1.00	23.51
3196	CD	GLU	A	228	79.737	68.868	6.911	1.00	25.72
3197	OE1	GLU	A	228	80.292	68.333	7.899	1.00	25.16
3198	OE2	GLU	A	228	80.367	69.272	5.910	1.00	28.53
3199	C	GLU	A	228	75.411	69.428	4.340	1.00	21.53
3200	O	GLU	A	228	74.644	70.370	4.532	1.00	22.09
3201	N	SER	A	229	75.600	68.899	3.141	1.00	21.49
3203	CA	SER	A	229	74.922	69.459	1.985	1.00	21.57
3205	CB	SER	A	229	75.598	69.036	0.695	1.00	21.17
3208	OG	SER	A	229	76.870	69.647	0.589	1.00	22.38

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3210	C	SER	A	229	73.432	69.119	1.967	1.00	21.32
3211	O	SER	A	229	72.629	69.993	1.719	1.00	20.51
3212	N	ILE	A	230	73.044	67.871	2.238	1.00	21.52
3214	CA	ILE	A	230	71.610	67.562	2.236	1.00	21.70
3216	CB	ILE	A	230	71.318	66.049	2.154	1.00	21.58
3218	CG1	ILE	A	230	71.881	65.279	3.347	1.00	22.85
3221	CD1	ILE	A	230	71.069	64.038	3.669	1.00	22.81
3225	CG2	ILE	A	230	71.815	65.486	0.849	1.00	21.97
3229	C	ILE	A	230	70.874	68.190	3.421	1.00	21.12
3230	O	ILE	A	230	69.684	68.467	3.337	1.00	21.31
3231	N	GLY	A	231	71.583	68.412	4.520	1.00	21.08
3233	CA	GLY	A	231	70.983	68.977	5.714	1.00	21.32
3236	C	GLY	A	231	70.607	70.441	5.534	1.00	21.14
3237	O	GLY	A	231	69.514	70.877	5.917	1.00	21.86
3238	N	LEU	A	232	71.513	71.205	4.939	1.00	21.35
3240	CA	LEU	A	232	71.214	72.583	4.595	1.00	21.18
3242	CB	LEU	A	232	72.467	73.318	4.127	1.00	21.49
3245	CG	LEU	A	232	72.250	74.769	3.712	1.00	21.63
3247	CD1	LEU	A	232	71.601	75.564	4.829	1.00	22.56
3251	CD2	LEU	A	232	73.571	75.361	3.320	1.00	23.37
3255	C	LEU	A	232	70.134	72.604	3.521	1.00	20.95
3256	O	LEU	A	232	69.171	73.324	3.659	1.00	20.57
3257	N	ALA	A	233	70.270	71.766	2.488	1.00	20.80
3259	CA	ALA	A	233	69.271	71.677	1.424	1.00	20.94
3261	CB	ALA	A	233	69.674	70.639	0.373	1.00	21.23
3265	C	ALA	A	233	67.885	71.350	1.966	1.00	20.81
3266	O	ALA	A	233	66.878	71.812	1.442	1.00	20.67
3267	N	PHE	A	234	67.840	70.554	3.029	1.00	20.67
3269	CA	PHE	A	234	66.568	70.166	3.634	1.00	20.70
3271	CB	PHE	A	234	66.798	69.201	4.785	1.00	20.78
3274	CG	PHE	A	234	65.600	68.375	5.131	1.00	22.14
3275	CD1	PHE	A	234	65.546	67.041	4.768	1.00	23.74
3277	CE1	PHE	A	234	64.455	66.267	5.103	1.00	25.17
3279	CZ	PHE	A	234	63.407	66.817	5.797	1.00	23.85
3281	CE2	PHE	A	234	63.462	68.143	6.173	1.00	23.26
3283	CD2	PHE	A	234	64.551	68.907	5.851	1.00	21.11
3285	C	PHE	A	234	65.812	71.378	4.147	1.00	20.30
3286	O	PHE	A	234	64.590	71.496	3.939	1.00	19.63
3287	N	GLN	A	235	66.523	72.269	4.835	1.00	20.63
3289	CA	GLN	A	235	65.874	73.456	5.381	1.00	21.12
3291	CB	GLN	A	235	66.699	74.091	6.503	1.00	21.39
3294	CG	GLN	A	235	65.944	75.205	7.276	1.00	21.45
3297	CD	GLN	A	235	64.668	74.715	7.926	1.00	23.00
3298	OE1	GLN	A	235	64.650	73.654	8.548	1.00	23.23
3299	NE2	GLN	A	235	63.595	75.490	7.795	1.00	20.99
3302	C	GLN	A	235	65.546	74.494	4.300	1.00	21.77
3303	O	GLN	A	235	64.511	75.148	4.375	1.00	22.39
3304	N	VAL	A	236	66.402	74.641	3.299	1.00	22.51
3306	CA	VAL	A	236	66.066	75.543	2.184	1.00	22.92
3308	CB	VAL	A	236	67.260	75.840	1.212	1.00	23.27
3310	CG1	VAL	A	236	68.054	74.664	0.922	1.00	26.25
3314	CG2	VAL	A	236	66.794	76.486	-0.102	1.00	23.71

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3318	C	VAL	A	236	64.794	75.075	1.478	1.00	22.84
3319	O	VAL	A	236	63.936	75.893	1.150	1.00	22.34
3320	N	GLN	A	237	64.635	73.761	1.307	1.00	23.02
3322	CA	GLN	A	237	63.413	73.222	0.738	1.00	23.04
3324	CB	GLN	A	237	63.538	71.727	0.418	1.00	23.87
3327	CG	GLN	A	237	62.276	71.128	-0.198	1.00	25.59
3330	CD	GLN	A	237	62.058	71.593	-1.623	1.00	29.42
3331	OE1	GLN	A	237	62.818	72.426	-2.133	1.00	30.57
3332	NE2	GLN	A	237	61.025	71.053	-2.275	1.00	28.29
3335	C	GLN	A	237	62.241	73.441	1.671	1.00	22.23
3336	O	GLN	A	237	61.140	73.709	1.213	1.00	22.37
3337	N	ASP	A	238	62.467	73.315	2.977	1.00	21.60
3339	CA	ASP	A	238	61.409	73.564	3.954	1.00	21.14
3341	CB	ASP	A	238	61.898	73.263	5.372	1.00	20.81
3344	CG	ASP	A	238	60.808	73.400	6.393	1.00	20.15
3345	OD1	ASP	A	238	59.877	72.588	6.376	1.00	22.40
3346	OD2	ASP	A	238	60.774	74.310	7.250	1.00	23.26
3347	C	ASP	A	238	60.904	75.018	3.848	1.00	21.37
3348	O	ASP	A	238	59.701	75.260	3.866	1.00	21.86
3349	N	ASP	A	239	61.820	75.966	3.694	1.00	21.89
3351	CA	ASP	A	239	61.446	77.379	3.534	1.00	22.75
3353	CB	ASP	A	239	62.674	78.275	3.478	1.00	22.66
3356	CG	ASP	A	239	63.436	78.375	4.789	1.00	23.92
3357	OD1	ASP	A	239	62.965	77.899	5.859	1.00	26.27
3358	OD2	ASP	A	239	64.542	78.966	4.821	1.00	23.49
3359	C	ASP	A	239	60.679	77.596	2.219	1.00	23.14
3360	O	ASP	A	239	59.719	78.357	2.158	1.00	23.09
3361	N	ILE	A	240	61.129	76.934	1.162	1.00	24.22
3363	CA	ILE	A	240	60.507	77.067	-0.150	1.00	24.50
3365	CB	ILE	A	240	61.358	76.356	-1.230	1.00	24.79
3367	CG1	ILE	A	240	62.593	77.200	-1.545	1.00	25.00
3370	CD1	ILE	A	240	63.697	76.444	-2.246	1.00	25.62
3374	CG2	ILE	A	240	60.548	76.118	-2.518	1.00	24.83
3378	C	ILE	A	240	59.094	76.529	-0.095	1.00	24.74
3379	O	ILE	A	240	58.168	77.162	-0.598	1.00	24.41
3380	N	LEU	A	241	58.920	75.380	0.561	1.00	24.90
3382	CA	LEU	A	241	57.608	74.763	0.702	1.00	25.47
3384	CB	LEU	A	241	57.721	73.376	1.346	1.00	25.41
3387	CG	LEU	A	241	58.364	72.296	0.469	1.00	26.20
3389	CD1	LEU	A	241	58.592	71.012	1.275	1.00	26.19
3393	CD2	LEU	A	241	57.523	72.032	-0.762	1.00	26.28
3397	C	LEU	A	241	56.677	75.637	1.517	1.00	25.82
3398	O	LEU	A	241	55.463	75.646	1.296	1.00	26.02
3399	N	ASP	A	242	57.238	76.375	2.461	1.00	26.06
3401	CA	ASP	A	242	56.422	77.233	3.298	1.00	27.02
3403	CB	ASP	A	242	57.239	77.832	4.426	1.00	26.69
3406	CG	ASP	A	242	56.390	78.176	5.607	1.00	28.82
3407	OD1	ASP	A	242	55.886	79.319	5.636	1.00	29.75
3408	OD2	ASP	A	242	56.148	77.365	6.534	1.00	31.49
3409	C	ASP	A	242	55.765	78.333	2.458	1.00	27.65
3410	O	ASP	A	242	54.622	78.689	2.698	1.00	28.08
3411	N	VAL	A	243	56.481	78.823	1.454	1.00	28.57

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3413	CA	VAL A	243		55.949	79.838	0.542	1.00	29.59
3415	CB	VAL A	243		57.091	80.577	-0.188	1.00	29.49
3417	CG1	VAL A	243		56.537	81.656	-1.140	1.00	29.98
3421	CG2	VAL A	243		58.062	81.200	0.825	1.00	29.51
3425	C	VAL A	243		54.951	79.248	-0.477	1.00	30.63
3426	O	VAL A	243		53.791	79.669	-0.525	1.00	30.78
3427	N	VAL A	244		55.388	78.253	-1.250	1.00	31.44
3429	CA	VAL A	244		54.642	77.785	-2.427	1.00	32.17
3431	CB	VAL A	244		55.605	77.525	-3.617	1.00	32.40
3433	CG1	VAL A	244		56.588	78.680	-3.768	1.00	32.66
3437	CG2	VAL A	244		56.349	76.185	-3.462	1.00	32.82
3441	C	VAL A	244		53.766	76.543	-2.233	1.00	32.47
3442	O	VAL A	244		52.963	76.204	-3.110	1.00	32.70
3443	N	GLY A	245		53.915	75.854	-1.105	1.00	32.77
3445	CA	GLY A	245		53.200	74.611	-0.879	1.00	33.14
3448	C	GLY A	245		51.784	74.871	-0.407	1.00	33.82
3449	O	GLY A	245		51.515	75.920	0.162	1.00	34.10
3450	N	ASP A	246		50.887	73.920	-0.656	1.00	34.38
3452	CA	ASP A	246		49.489	73.995	-0.211	1.00	34.75
3454	CB	ASP A	246		48.602	73.159	-1.151	1.00	35.30
3457	CG	ASP A	246		47.185	73.699	-1.272	1.00	38.65
3458	OD1	ASP A	246		46.738	73.925	-2.425	1.00	42.04
3459	OD2	ASP A	246		46.433	73.914	-0.284	1.00	42.91
3460	C	ASP A	246		49.431	73.410	1.198	1.00	33.97
3461	O	ASP A	246		50.088	72.411	1.456	1.00	33.79
3462	N	THR A	247		48.643	74.009	2.089	1.00	33.08
3464	CA	THR A	247		48.489	73.517	3.465	1.00	32.87
3466	CB	THR A	247		47.476	74.394	4.249	1.00	32.46
3468	OG1	THR A	247		48.002	75.710	4.420	1.00	32.70
3470	CG2	THR A	247		47.288	73.901	5.684	1.00	32.42
3474	C	THR A	247		48.061	72.041	3.542	1.00	32.67
3475	O	THR A	247		48.561	71.297	4.377	1.00	32.65
3476	N	ALA A	248		47.141	71.617	2.677	1.00	32.34
3478	CA	ALA A	248		46.651	70.240	2.709	1.00	32.14
3480	CB	ALA A	248		45.388	70.095	1.857	1.00	32.51
3484	C	ALA A	248		47.724	69.228	2.271	1.00	31.60
3485	O	ALA A	248		47.692	68.073	2.678	1.00	31.38
3486	N	THR A	249		48.668	69.666	1.447	1.00	31.12
3488	CA	THR A	249		49.785	68.815	1.025	1.00	31.09
3490	CB	THR A	249		50.269	69.251	-0.371	1.00	31.32
3492	OG1	THR A	249		49.192	69.112	-1.313	1.00	33.79
3494	CG2	THR A	249		51.348	68.308	-0.917	1.00	31.41
3498	C	THR A	249		50.943	68.825	2.045	1.00	30.23
3499	O	THR A	249		51.483	67.768	2.391	1.00	30.03
3500	N	LEU A	250		51.312	70.017	2.520	1.00	29.30
3502	CA	LEU A	250		52.358	70.175	3.539	1.00	28.64
3504	CB	LEU A	250		52.668	71.653	3.766	1.00	28.31
3507	CG	LEU A	250		53.253	72.412	2.577	1.00	29.19
3509	CD1	LEU A	250		53.329	73.903	2.883	1.00	29.07
3513	CD2	LEU A	250		54.620	71.880	2.197	1.00	29.56
3517	C	LEU A	250		52.007	69.554	4.880	1.00	27.73
3518	O	LEU A	250		52.877	69.038	5.578	1.00	27.92

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3519	N	GLY	A	251	50.732	69.613	5.240	1.00	26.76
3521	CA	GLY	A	251	50.277	69.195	6.546	1.00	26.19
3524	C	GLY	A	251	50.485	70.266	7.601	1.00	25.80
3525	O	GLY	A	251	50.150	70.053	8.757	1.00	24.95
3526	N	LYS	A	252	51.071	71.388	7.197	1.00	25.86
3528	CA	LYS	A	252	51.273	72.556	8.052	1.00	26.53
3530	CB	LYS	A	252	52.701	72.588	8.628	1.00	25.80
3533	CG	LYS	A	252	53.804	72.498	7.579	1.00	25.64
3536	CD	LYS	A	252	55.183	72.231	8.200	1.00	23.61
3539	CE	LYS	A	252	56.297	72.507	7.205	1.00	22.86
3542	NZ	LYS	A	252	57.604	71.866	7.602	1.00	21.94
3546	C	LYS	A	252	50.992	73.813	7.223	1.00	27.55
3547	O	LYS	A	252	51.046	73.781	5.982	1.00	28.12
3548	N	ARG	A	253	50.721	74.918	7.905	1.00	28.61
3550	CA	ARG	A	253	50.217	76.128	7.249	1.00	29.63
3552	CB	ARG	A	253	49.658	77.096	8.287	1.00	30.10
3555	CG	ARG	A	253	48.370	76.612	8.875	1.00	32.12
3558	CD	ARG	A	253	47.441	77.693	9.362	1.00	35.28
3561	NE	ARG	A	253	46.380	77.104	10.175	1.00	38.07
3563	CZ	ARG	A	253	45.308	76.476	9.688	1.00	40.08
3564	NH1	ARG	A	253	45.095	76.378	8.376	1.00	39.60
3567	NH2	ARG	A	253	44.419	75.962	10.533	1.00	40.97
3570	C	ARG	A	253	51.223	76.852	6.360	1.00	29.71
3571	O	ARG	A	253	52.306	77.274	6.806	1.00	29.38
3572	N	GLN	A	254	50.847	76.966	5.084	1.00	30.10
3574	CA	GLN	A	254	51.544	77.794	4.108	1.00	29.94
3576	CB	GLN	A	254	50.816	77.731	2.754	1.00	30.17
3579	CG	GLN	A	254	51.436	78.643	1.649	1.00	31.83
3582	CD	GLN	A	254	50.618	78.716	0.357	1.00	34.25
3583	OE1	GLN	A	254	51.157	79.057	-0.705	1.00	35.57
3584	NE2	GLN	A	254	49.333	78.396	0.439	1.00	35.68
3587	C	GLN	A	254	51.586	79.238	4.601	1.00	29.79
3588	O	GLN	A	254	50.625	79.733	5.193	1.00	29.82
3589	N	GLY	A	255	52.705	79.907	4.369	1.00	29.23
3591	CA	GLY	A	255	52.843	81.298	4.740	1.00	29.36
3594	C	GLY	A	255	53.063	81.513	6.230	1.00	29.17
3595	O	GLY	A	255	52.963	82.630	6.708	1.00	28.41
3596	N	ALA	A	256	53.372	80.453	6.971	1.00	29.32
3598	CA	ALA	A	256	53.670	80.594	8.395	1.00	29.31
3600	CB	ALA	A	256	53.865	79.216	9.032	1.00	29.54
3604	C	ALA	A	256	54.900	81.481	8.638	1.00	29.48
3605	O	ALA	A	256	54.915	82.276	9.569	1.00	30.09
3606	N	ASP	A	257	55.925	81.350	7.805	1.00	29.41
3608	CA	ASP	A	257	57.170	82.079	8.006	1.00	29.43
3610	CB	ASP	A	257	58.242	81.581	7.053	1.00	29.35
3613	CG	ASP	A	257	58.770	80.208	7.420	1.00	28.93
3614	OD1	ASP	A	257	58.493	79.724	8.552	1.00	27.10
3615	OD2	ASP	A	257	59.480	79.562	6.613	1.00	25.07
3616	C	ASP	A	257	56.992	83.576	7.772	1.00	30.15
3617	O	ASP	A	257	57.516	84.404	8.505	1.00	28.74
3618	N	GLN	A	258	56.258	83.887	6.717	1.00	31.27
3620	CA	GLN	A	258	56.003	85.254	6.311	1.00	32.11

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3622	CB	BGLN	A	258	55.223	85.271	4.997	0.35	32.00
3623	CB	AGLN	A	258	55.313	85.259	4.930	0.65	32.18
3628	CG	BGLN	A	258	55.115	86.632	4.342	0.35	31.76
3629	CG	AGLN	A	258	56.317	84.920	3.801	0.65	32.43
3634	CD	BGLN	A	258	54.771	86.519	2.876	0.35	31.23
3635	CD	AGLN	A	258	55.724	84.264	2.547	0.65	32.97
3636	OE1	BGLN	A	258	55.645	86.639	2.016	0.35	30.93
3637	OE1	AGLN	A	258	54.977	83.279	2.618	0.65	32.08
3638	NE2	BGLN	A	258	53.503	86.266	2.585	0.35	30.18
3639	NE2	AGLN	A	258	56.103	84.792	1.389	0.65	33.37
3644	C	GLN	A	258	55.203	85.967	7.400	1.00	32.82
3645	O	GLN	A	258	55.460	87.123	7.720	1.00	33.46
3646	N	GLN	A	259	54.266	85.249	8.000	1.00	33.70
3648	CA	GLN	A	259	53.452	85.780	9.084	1.00	34.64
3650	CB	GLN	A	259	52.395	84.756	9.463	1.00	35.35
3653	CG	GLN	A	259	51.346	85.257	10.436	1.00	38.57
3656	CD	GLN	A	259	50.161	84.331	10.482	1.00	42.61
3657	OE1	GLN	A	259	49.161	84.555	9.787	1.00	45.33
3658	NE2	GLN	A	259	50.272	83.263	11.278	1.00	44.63
3661	C	GLN	A	259	54.281	86.173	10.320	1.00	34.20
3662	O	GLN	A	259	53.948	87.154	10.990	1.00	33.93
3663	N	LEU	A	260	55.347	85.419	10.613	1.00	33.21
3665	CA	LEU	A	260	56.247	85.737	11.734	1.00	32.74
3667	CB	LEU	A	260	56.676	84.463	12.474	1.00	32.73
3670	CG	LEU	A	260	55.629	83.549	13.112	1.00	34.09
3672	CD1	LEU	A	260	56.300	82.734	14.206	1.00	35.07
3676	CD2	LEU	A	260	54.412	84.295	13.676	1.00	35.20
3680	C	LEU	A	260	57.514	86.495	11.326	1.00	31.74
3681	O	LEU	A	260	58.348	86.790	12.172	1.00	31.90
3682	N	GLY	A	261	57.670	86.808	10.043	1.00	30.66
3684	CA	GLY	A	261	58.858	87.495	9.565	1.00	29.51
3687	C	GLY	A	261	60.157	86.732	9.759	1.00	28.74
3688	O	GLY	A	261	61.198	87.333	9.998	1.00	28.52
3689	N	LYS	A	262	60.099	85.405	9.649	1.00	27.62
3691	CA	LYS	A	262	61.296	84.575	9.707	1.00	26.77
3693	CB	LYS	A	262	60.934	83.092	9.572	1.00	26.29
3696	CG	LYS	A	262	60.021	82.536	10.642	1.00	25.90
3699	CD	LYS	A	262	60.797	82.141	11.884	1.00	26.17
3702	CE	LYS	A	262	59.882	81.593	12.965	1.00	26.68
3705	NZ	LYS	A	262	60.644	81.319	14.214	1.00	25.74
3709	C	LYS	A	262	62.280	84.943	8.595	1.00	26.39
3710	O	LYS	A	262	61.884	85.161	7.445	1.00	26.03
3711	N	SER	A	263	63.563	85.005	8.943	1.00	26.23
3713	CA	SER	A	263	64.629	85.019	7.944	1.00	26.10
3715	CB	SER	A	263	65.975	85.311	8.586	1.00	26.43
3718	OG	SER	A	263	65.979	86.581	9.207	1.00	26.96
3720	C	SER	A	263	64.666	83.652	7.247	1.00	26.21
3721	O	SER	A	263	64.899	82.629	7.898	1.00	25.19
3722	N	THR	A	264	64.388	83.642	5.942	1.00	25.65
3724	CA	THR	A	264	64.408	82.408	5.149	1.00	25.89
3726	CB	THR	A	264	62.975	81.922	4.812	1.00	26.14
3728	OG1	THR	A	264	62.368	82.789	3.847	1.00	26.91

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3730	CG2	THR A	264		62.046	81.992	6.033	1.00	26.45
3734	C	THR A	264		65.189	82.591	3.856	1.00	25.77
3735	O	THR A	264		65.538	83.722	3.472	1.00	25.52
3736	N	TYR A	265		65.479	81.471	3.195	1.00	25.31
3738	CA	TYR A	265		66.114	81.507	1.886	1.00	25.24
3740	CB	TYR A	265		66.555	80.104	1.428	1.00	24.84
3743	CG	TYR A	265		67.953	79.767	1.902	1.00	24.29
3744	CD1	TYR A	265		69.012	79.698	1.010	1.00	23.63
3746	CE1	TYR A	265		70.282	79.407	1.423	1.00	24.04
3748	CZ	TYR A	265		70.545	79.200	2.759	1.00	24.29
3749	OH	TYR A	265		71.827	78.928	3.168	1.00	24.41
3751	CE2	TYR A	265		69.521	79.276	3.685	1.00	24.92
3753	CD2	TYR A	265		68.225	79.566	3.250	1.00	23.77
3755	C	TYR A	265		65.240	82.222	0.843	1.00	25.25
3756	O	TYR A	265		65.717	83.149	0.211	1.00	25.83
3757	N	PRO A	266		63.982	81.823	0.658	1.00	25.61
3758	CA	PRO A	266		63.108	82.515	-0.307	1.00	25.70
3760	CB	PRO A	266		61.812	81.700	-0.284	1.00	26.04
3763	CG	PRO A	266		61.876	80.854	0.923	1.00	26.04
3766	CD	PRO A	266		63.311	80.683	1.293	1.00	25.37
3769	C	PRO A	266		62.825	83.980	0.027	1.00	25.95
3770	O	PRO A	266		62.702	84.784	-0.900	1.00	25.00
3771	N	ALA A	267		62.738	84.326	1.311	1.00	26.04
3773	CA	ALA A	267		62.503	85.719	1.697	1.00	26.33
3775	CB	ALA A	267		62.193	85.853	3.166	1.00	26.37
3779	C	ALA A	267		63.694	86.578	1.309	1.00	26.47
3780	O	ALA A	267		63.512	87.637	0.734	1.00	26.90
3781	N	LEU A	268		64.906	86.094	1.574	1.00	26.35
3783	CA	LEU A	268		66.124	86.814	1.213	1.00	26.27
3785	CB	LEU A	268		67.337	86.201	1.924	1.00	26.30
3788	CG	LEU A	268		68.691	86.873	1.690	1.00	27.65
3790	CD1	LEU A	268		68.728	88.322	2.211	1.00	28.07
3794	CD2	LEU A	268		69.803	86.053	2.316	1.00	28.26
3798	C	LEU A	268		66.386	86.828	-0.294	1.00	26.01
3799	O	LEU A	268		66.541	87.899	-0.898	1.00	25.44
3800	N	LEU A	269		66.439	85.633	-0.881	1.00	25.58
3802	CA	LEU A	269		66.963	85.430	-2.234	1.00	25.43
3804	CB	LEU A	269		67.755	84.113	-2.298	1.00	25.44
3807	CG	LEU A	269		68.906	83.896	-1.320	1.00	26.67
3809	CD1	LEU A	269		69.520	82.486	-1.510	1.00	25.96
3813	CD2	LEU A	269		69.960	84.976	-1.479	1.00	27.24
3817	C	LEU A	269		65.902	85.380	-3.316	1.00	24.91
3818	O	LEU A	269		66.226	85.454	-4.490	1.00	24.92
3819	N	GLY A	270		64.640	85.253	-2.933	1.00	24.87
3821	CA	GLY A	270		63.584	84.945	-3.884	1.00	24.94
3824	C	GLY A	270		63.529	83.446	-4.151	1.00	25.33
3825	O	GLY A	270		64.488	82.724	-3.871	1.00	25.08
3826	N	LEU A	271		62.415	82.985	-4.699	1.00	25.79
3828	CA	LEU A	271		62.170	81.567	-4.899	1.00	26.67
3830	CB	LEU A	271		60.732	81.320	-5.383	1.00	27.35
3833	CG	LEU A	271		59.602	81.477	-4.365	1.00	28.42
3835	CD1	LEU A	271		58.252	81.403	-5.068	1.00	29.93

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3839	CD2	LEU	A	271	59.687	80.413	-3.279	1.00	28.63
3843	C	LEU	A	271	63.162	80.914	-5.853	1.00	27.13
3844	O	LEU	A	271	63.593	79.796	-5.591	1.00	27.11
3845	N	GLU	A	272	63.536	81.599	-6.938	1.00	27.48
3847	CA	GLU	A	272	64.429	81.018	-7.956	1.00	28.05
3849	CB	GLU	A	272	64.488	81.905	-9.229	1.00	28.98
3852	CG	GLU	A	272	65.687	81.611	-10.148	1.00	31.69
3855	CD	GLU	A	272	65.592	82.253	-11.528	1.00	35.38
3856	OE1	GLU	A	272	66.103	81.648	-12.499	1.00	39.00
3857	OE2	GLU	A	272	65.013	83.354	-11.655	1.00	37.35
3858	C	GLU	A	272	65.850	80.739	-7.455	1.00	27.43
3859	O	GLU	A	272	66.427	79.668	-7.745	1.00	27.14
3860	N	GLN	A	273	66.432	81.697	-6.743	1.00	26.16
3862	CA	GLN	A	273	67.799	81.563	-6.250	1.00	26.17
3864	CB	GLN	A	273	68.364	82.909	-5.793	1.00	26.14
3867	CG	GLN	A	273	68.642	83.881	-6.920	1.00	29.26
3870	CD	GLN	A	273	69.025	85.266	-6.418	1.00	32.23
3871	OE1	GLN	A	273	69.828	85.405	-5.485	1.00	34.54
3872	NE2	GLN	A	273	68.464	86.295	-7.046	1.00	34.59
3875	C	GLN	A	273	67.854	80.566	-5.092	1.00	25.40
3876	O	GLN	A	273	68.856	79.905	-4.900	1.00	25.15
3877	N	ALA	A	274	66.776	80.485	-4.318	1.00	25.33
3879	CA	ALA	A	274	66.681	79.514	-3.239	1.00	25.32
3881	CB	ALA	A	274	65.429	79.770	-2.427	1.00	25.59
3885	C	ALA	A	274	66.665	78.097	-3.837	1.00	25.68
3886	O	ALA	A	274	67.388	77.213	-3.385	1.00	25.35
3887	N	ARG	A	275	65.860	77.913	-4.878	1.00	25.78
3889	CA	ARG	A	275	65.753	76.631	-5.564	1.00	26.49
3891	CB	ARG	A	275	64.725	76.697	-6.683	1.00	26.59
3894	CG	ARG	A	275	63.311	76.604	-6.197	1.00	27.19
3897	CD	ARG	A	275	62.284	76.791	-7.294	1.00	29.91
3900	NE	ARG	A	275	60.926	76.575	-6.799	1.00	31.85
3902	CZ	ARG	A	275	59.886	77.379	-7.009	1.00	34.22
3903	NH1	ARG	A	275	59.998	78.504	-7.720	1.00	35.16
3906	NH2	ARG	A	275	58.706	77.047	-6.491	1.00	35.99
3909	C	ARG	A	275	67.091	76.201	-6.109	1.00	26.94
3910	O	ARG	A	275	67.468	75.039	-5.985	1.00	27.03
3911	N	LYS	A	276	67.816	77.155	-6.679	1.00	27.58
3913	CA	LYS	A	276	69.145	76.929	-7.218	1.00	28.35
3915	CB	LYS	A	276	69.641	78.193	-7.934	1.00	29.25
3918	CG	LYS	A	276	71.101	78.163	-8.408	1.00	31.10
3921	CD	LYS	A	276	71.288	77.283	-9.637	1.00	34.04
3924	CE	LYS	A	276	72.514	77.689	-10.473	1.00	35.05
3927	NZ	LYS	A	276	73.803	77.493	-9.748	1.00	35.48
3931	C	LYS	A	276	70.130	76.552	-6.132	1.00	28.37
3932	O	LYS	A	276	70.987	75.692	-6.347	1.00	28.80
3933	N	LYS	A	277	70.054	77.222	-4.986	1.00	28.08
3935	CA	LYS	A	277	70.938	76.890	-3.873	1.00	27.92
3937	CB	LYS	A	277	70.723	77.824	-2.675	1.00	28.22
3940	CG	LYS	A	277	71.163	79.279	-2.921	1.00	30.08
3943	CD	LYS	A	277	72.546	79.581	-2.376	1.00	31.98
3946	CE	LYS	A	277	72.871	81.085	-2.414	1.00	32.86

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3949	NZ	LYS	A	277	74.277	81.323	-2.846	1.00	33.80
3953	C	LYS	A	277	70.680	75.438	-3.453	1.00	27.24
3954	O	LYS	A	277	71.620	74.699	-3.201	1.00	26.52
3955	N	ALA	A	278	69.411	75.041	-3.393	1.00	26.71
3957	CA	ALA	A	278	69.053	73.682	-2.960	1.00	26.99
3959	CB	ALA	A	278	67.544	73.546	-2.823	1.00	26.84
3963	C	ALA	A	278	69.589	72.651	-3.949	1.00	27.26
3964	O	ALA	A	278	70.141	71.636	-3.566	1.00	26.69
3965	N	ARG	A	279	69.427	72.948	-5.234	1.00	27.61
3967	CA	ARG	A	279	69.869	72.070	-6.311	1.00	28.16
3969	CB	ARG	A	279	69.332	72.603	-7.641	1.00	28.87
3972	CG	ARG	A	279	69.910	71.996	-8.886	1.00	32.19
3975	CD	ARG	A	279	69.160	72.414	-10.158	1.00	35.33
3978	NE	ARG	A	279	68.039	73.319	-9.871	1.00	38.00
3980	CZ	ARG	A	279	68.005	74.632	-10.133	1.00	38.95
3981	NH1	ARG	A	279	69.027	75.256	-10.711	1.00	40.27
3984	NH2	ARG	A	279	66.924	75.329	-9.815	1.00	38.71
3987	C	ARG	A	279	71.389	71.923	-6.336	1.00	27.24
3988	O	ARG	A	279	71.885	70.819	-6.512	1.00	27.02
3989	N	ASP	A	280	72.116	73.021	-6.128	1.00	26.36
3991	CA	ASP	A	280	73.586	72.995	-6.059	1.00	25.90
3993	CB	ASP	A	280	74.150	74.420	-6.005	1.00	26.39
3996	CG	ASP	A	280	74.006	75.175	-7.335	1.00	28.03
3997	OD1	ASP	A	280	74.090	76.423	-7.315	1.00	30.25
3998	OD2	ASP	A	280	73.790	74.623	-8.433	1.00	28.83
3999	C	ASP	A	280	74.086	72.217	-4.828	1.00	25.37
4000	O	ASP	A	280	75.128	71.557	-4.873	1.00	24.74
4001	N	LEU	A	281	73.346	72.307	-3.727	1.00	24.45
4003	CA	LEU	A	281	73.688	71.553	-2.529	1.00	24.47
4005	CB	LEU	A	281	72.825	71.999	-1.335	1.00	24.55
4008	CG	LEU	A	281	73.246	73.324	-0.700	1.00	23.94
4010	CD1	LEU	A	281	72.129	73.904	0.129	1.00	23.80
4014	CD2	LEU	A	281	74.506	73.133	0.150	1.00	23.78
4018	C	LEU	A	281	73.526	70.048	-2.781	1.00	24.25
4019	O	LEU	A	281	74.364	69.262	-2.353	1.00	23.54
4020	N	ILE	A	282	72.459	69.660	-3.475	1.00	24.75
4022	CA	ILE	A	282	72.221	68.242	-3.788	1.00	25.66
4024	CB	ILE	A	282	70.771	67.998	-4.289	1.00	25.32
4026	CG1	ILE	A	282	69.745	68.291	-3.185	1.00	25.41
4029	CD1	ILE	A	282	70.153	67.917	-1.800	1.00	25.34
4033	CG2	ILE	A	282	70.592	66.548	-4.826	1.00	25.27
4037	C	ILE	A	282	73.241	67.719	-4.788	1.00	26.42
4038	O	ILE	A	282	73.728	66.602	-4.641	1.00	26.98
4039	N	ASP	A	283	73.571	68.511	-5.802	1.00	27.38
4041	CA	ASP	A	283	74.607	68.111	-6.753	1.00	28.16
4043	CB	ASP	A	283	74.799	69.165	-7.851	1.00	28.99
4046	CG	ASP	A	283	73.578	69.319	-8.758	1.00	31.72
4047	OD1	ASP	A	283	73.510	70.341	-9.477	1.00	36.96
4048	OD2	ASP	A	283	72.644	68.493	-8.830	1.00	35.17
4049	C	ASP	A	283	75.929	67.903	-5.997	1.00	27.86
4050	O	ASP	A	283	76.696	67.003	-6.319	1.00	27.48
4051	N	ASP	A	284	76.189	68.740	-4.988	1.00	27.56

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4053	CA	ASP A	284		77.405	68.623	-4.177	1.00	27.43
4055	CB	ASP A	284		77.573	69.869	-3.296	1.00	27.98
4058	CG	ASP A	284		78.753	69.774	-2.351	1.00	29.55
4059	OD1	ASP A	284		79.871	70.166	-2.754	1.00	34.48
4060	OD2	ASP A	284		78.662	69.347	-1.179	1.00	30.96
4061	C	ASP A	284		77.344	67.351	-3.320	1.00	26.91
4062	O	ASP A	284		78.347	66.666	-3.137	1.00	26.70
4063	N	ALA A	285		76.154	67.039	-2.817	1.00	26.35
4065	CA	ALA A	285		75.935	65.830	-2.041	1.00	26.26
4067	CB	ALA A	285		74.514	65.811	-1.452	1.00	26.18
4071	C	ALA A	285		76.164	64.607	-2.913	1.00	26.41
4072	O	ALA A	285		76.774	63.648	-2.469	1.00	26.46
4073	N	ARG A	286		75.687	64.647	-4.156	1.00	26.93
4075	CA	ARG A	286		75.888	63.543	-5.095	1.00	27.77
4077	CB	ARG A	286		75.153	63.778	-6.413	1.00	28.06
4080	CG	ARG A	286		73.650	63.500	-6.353	1.00	30.42
4083	CD	ARG A	286		72.949	63.511	-7.727	1.00	33.16
4086	NE	ARG A	286		71.739	62.694	-7.695	1.00	35.04
4088	CZ	ARG A	286		71.709	61.365	-7.828	1.00	37.56
4089	NH1	ARG A	286		72.820	60.653	-8.041	1.00	37.77
4092	NH2	ARG A	286		70.544	60.731	-7.757	1.00	37.95
4095	C	ARG A	286		77.377	63.333	-5.364	1.00	28.02
4096	O	ARG A	286		77.837	62.202	-5.438	1.00	27.64
4097	N	GLN A	287		78.120	64.427	-5.478	1.00	28.41
4099	CA	GLN A	287		79.550	64.352	-5.768	1.00	29.05
4101	CB	GLN A	287		80.163	65.742	-5.984	1.00	29.26
4104	CG	GLN A	287		79.870	66.348	-7.343	1.00	31.16
4107	CD	GLN A	287		80.342	65.469	-8.494	1.00	34.10
4108	OE1	GLN A	287		81.544	65.280	-8.687	1.00	36.57
4109	NE2	GLN A	287		79.396	64.921	-9.248	1.00	34.65
4112	C	GLN A	287		80.260	63.638	-4.645	1.00	28.84
4113	O	GLN A	287		81.060	62.747	-4.898	1.00	29.43
4114	N	SER A	288		79.946	64.002	-3.403	1.00	28.72
4116	CA	SER A	288		80.514	63.331	-2.234	1.00	28.70
4118	CB	SER A	288		79.948	63.912	-0.930	1.00	28.50
4121	OG	SER A	288		80.451	65.214	-0.693	1.00	28.19
4123	C	SER A	288		80.254	61.824	-2.255	1.00	28.86
4124	O	SER A	288		81.143	61.046	-1.948	1.00	28.79
4125	N	LEU A	289		79.028	61.428	-2.579	1.00	29.44
4127	CA	LEU A	289		78.666	60.005	-2.650	1.00	29.79
4129	CB	LEU A	289		77.163	59.818	-2.910	1.00	29.50
4132	CG	LEU A	289		76.184	60.273	-1.815	1.00	28.59
4134	CD1	LEU A	289		74.747	60.026	-2.249	1.00	28.94
4138	CD2	LEU A	289		76.473	59.585	-0.493	1.00	27.92
4142	C	LEU A	289		79.472	59.246	-3.717	1.00	30.81
4143	O	LEU A	289		79.732	58.062	-3.545	1.00	30.71
4144	N	LYS A	290		79.870	59.919	-4.800	1.00	31.59
4146	CA	LYS A	290		80.704	59.288	-5.837	1.00	32.26
4148	CB	LYS A	290		80.998	60.268	-6.989	1.00	32.55
4151	CG	LYS A	290		79.794	60.560	-7.898	1.00	34.13
4154	CD	LYS A	290		80.188	61.386	-9.153	1.00	35.23
4157	CE	LYS A	290		79.129	61.238	-10.259	1.00	36.81

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4160	NZ	LYS A	290		79.083	62.387	-11.229	1.00	37.86
4164	C	LYS A	290		82.012	58.741	-5.256	1.00	32.60
4165	O	LYS A	290		82.471	57.679	-5.650	1.00	33.03
4166	N	GLN A	291		82.589	59.462	-4.300	1.00	33.38
4168	CA	GLN A	291		83.796	59.026	-3.599	1.00	34.01
4170	CB	GLN A	291		84.253	60.103	-2.607	1.00	34.60
4173	CG	GLN A	291		84.614	61.448	-3.230	1.00	35.87
4176	CD	GLN A	291		85.108	62.446	-2.197	1.00	37.47
4177	OE1	GLN A	291		86.039	62.155	-1.446	1.00	39.36
4178	NE2	GLN A	291		84.483	63.615	-2.149	1.00	39.06
4181	C	GLN A	291		83.589	57.715	-2.830	1.00	34.18
4182	O	GLN A	291		84.513	56.909	-2.707	1.00	34.15
4183	N	LEU A	292		82.385	57.520	-2.294	1.00	33.99
4185	CA	LEU A	292		82.047	56.287	-1.591	1.00	34.26
4187	CB	LEU A	292		80.849	56.509	-0.670	1.00	33.95
4190	CG	LEU A	292		81.061	57.578	0.398	1.00	33.40
4192	CD1	LEU A	292		79.805	57.720	1.223	1.00	33.09
4196	CD2	LEU A	292		82.269	57.242	1.274	1.00	33.91
4200	C	LEU A	292		81.738	55.137	-2.533	1.00	34.79
4201	O	LEU A	292		82.073	53.989	-2.239	1.00	34.64
4202	N	ALA A	293		81.072	55.445	-3.642	1.00	35.56
4204	CA	ALA A	293		80.741	54.450	-4.660	1.00	36.49
4206	CB	ALA A	293		79.825	55.061	-5.712	1.00	36.38
4210	C	ALA A	293		82.012	53.886	-5.311	1.00	37.32
4211	O	ALA A	293		82.015	52.758	-5.799	1.00	37.70
4212	N	GLU A	294		83.075	54.690	-5.296	1.00	38.52
4214	CA	GLU A	294		84.421	54.297	-5.744	1.00	39.54
4216	CB	GLU A	294		85.353	55.513	-5.677	1.00	39.78
4219	CG	GLU A	294		86.404	55.572	-6.767	1.00	41.97
4222	CD	GLU A	294		86.407	56.897	-7.488	1.00	43.76
4223	OE1	GLU A	294		86.681	57.915	-6.825	1.00	46.66
4224	OE2	GLU A	294		86.129	56.921	-8.705	1.00	45.53
4225	C	GLU A	294		85.034	53.179	-4.895	1.00	39.49
4226	O	GLU A	294		85.883	52.422	-5.363	1.00	40.00
4227	N	GLN A	295		84.617	53.112	-3.638	1.00	39.43
4229	CA	GLN A	295		85.085	52.109	-2.700	1.00	39.30
4231	CB	GLN A	295		85.306	52.752	-1.324	1.00	39.51
4234	CG	GLN A	295		86.094	54.061	-1.348	1.00	40.85
4237	CD	GLN A	295		86.003	54.825	-0.033	1.00	42.68
4238	OE1	GLN A	295		85.958	54.217	1.037	1.00	44.83
4239	NE2	GLN A	295		85.983	56.156	-0.110	1.00	42.30
4242	C	GLN A	295		84.087	50.944	-2.594	1.00	38.62
4243	O	GLN A	295		84.083	50.210	-1.605	1.00	38.99
4244	N	SER A	296		83.250	50.794	-3.616	1.00	37.61
4246	CA	SER A	296		82.260	49.718	-3.721	1.00	36.98
4248	CB	SER A	296		82.963	48.362	-3.884	1.00	37.17
4251	OG	SER A	296		83.487	48.241	-5.197	1.00	38.77
4253	C	SER A	296		81.210	49.685	-2.598	1.00	35.68
4254	O	SER A	296		80.722	48.617	-2.206	1.00	35.55
4255	N	LEU A	297		80.867	50.865	-2.092	1.00	34.25
4257	CA	LEU A	297		79.710	51.032	-1.218	1.00	32.88
4259	CB	LEU A	297		79.997	52.090	-0.161	1.00	32.92

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4262	CG	LEU	A	297	81.178	51.793	0.755	1.00	33.21
4264	CD1	LEU	A	297	81.567	53.040	1.532	1.00	33.05
4268	CD2	LEU	A	297	80.872	50.609	1.704	1.00	33.61
4272	C	LEU	A	297	78.507	51.432	-2.074	1.00	31.66
4273	O	LEU	A	297	78.621	52.255	-2.988	1.00	31.32
4274	N	ASP	A	298	77.361	50.827	-1.799	1.00	30.63
4276	CA	ASP	A	298	76.127	51.123	-2.528	1.00	29.60
4278	CB	ASP	A	298	75.150	49.956	-2.371	1.00	29.83
4281	CG	ASP	A	298	73.911	50.089	-3.251	1.00	30.98
4282	OD1	ASP	A	298	73.673	51.177	-3.843	1.00	30.78
4283	OD2	ASP	Ä	298	73.117	49.135	-3.407	1.00	32.78
4284	C	ASP	A	298	75.516	52.431	-2.021	1.00	28.62
4285	O	ASP	A	298	74.919	52.474	-0.953	1.00	27.93
4286	N	THR	A	299	75.655	53.496	-2.801	1.00	27.78
4288	CA	THR	A	299	75.152	54.812	-2.395	1.00	27.48
4290	CB	THR	A	299	76.121	55.907	-2.850	1.00	27.79
4292	OG1	THR	A	299	76.198	55.923	-4.282	1.00	27.64
4294	CG2	THR	A	299	77.522	55.612	-2.397	1.00	27.86
4298	C	THR	A	299	73.775	55.130	-2.963	1.00	26.98
4299	O	THR	A	299	73.314	56.269	-2.852	1.00	26.90
4300	N	SER	A	300	73.115	54.136	-3.549	1.00	25.87
4302	CA	SER	A	300	71.884	54.371	-4.303	1.00	25.78
4304	CB	SER	A	300	71.469	53.116	-5.083	1.00	25.66
4307	OG	SER	A	300	71.181	52.042	-4.210	1.00	28.03
4309	C	SER	A	300	70.718	54.922	-3.460	1.00	24.86
4310	O	SER	A	300	69.989	55.799	-3.922	1.00	24.04
4311	N	ALA	A	301	70.538	54.423	-2.237	1.00	24.31
4313	CA	ALA	A	301	69.491	54.957	-1.356	1.00	23.85
4315	CB	ALA	A	301	69.266	54.058	-0.138	1.00	23.74
4319	C	ALA	A	301	69.813	56.402	-0.925	1.00	23.51
4320	O	ALA	A	301	68.927	57.234	-0.865	1.00	22.49
4321	N	LEU	A	302	71.082	56.696	-0.670	1.00	23.59
4323	CA	LEU	A	302	71.476	58.050	-0.254	1.00	24.04
4325	CB	LEU	A	302	72.893	58.059	0.321	1.00	23.68
4328	CG	LEU	A	302	73.047	57.380	1.677	1.00	24.07
4330	CD1	LEU	A	302	74.495	57.511	2.165	1.00	25.59
4334	CD2	LEU	A	302	72.085	57.972	2.680	1.00	24.26
4338	C	LEU	A	302	71.375	59.070	-1.370	1.00	24.05
4339	O	LEU	A	302	71.128	60.238	-1.104	1.00	24.30
4340	N	GLU	A	303	71.575	58.648	-2.614	1.00	24.92
4342	CA	GLU	A	303	71.455	59.578	-3.734	1.00	25.79
4344	CB	GLU	A	303	72.238	59.158	-4.988	1.00	26.38
4347	CG	GLU	A	303	72.152	57.732	-5.448	1.00	28.99
4350	CD	GLU	A	303	73.344	57.345	-6.333	1.00	31.29
4351	OE1	GLU	A	303	73.673	58.127	-7.247	1.00	31.21
4352	OE2	GLU	A	303	73.966	56.274	-6.098	1.00	33.39
4353	C	GLU	A	303	69.982	59.834	-4.045	1.00	25.52
4354	O	GLU	A	303	69.605	60.961	-4.347	1.00	25.13
4355	N	ALA	A	304	69.152	58.797	-3.927	1.00	25.73
4357	CA	ALA	A	304	67.709	58.953	-4.149	1.00	25.33
4359	CB	ALA	A	304	67.020	57.609	-4.201	1.00	25.75
4363	C	ALA	A	304	67.099	59.830	-3.059	1.00	25.32

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4364	O	ALA A	304		66.202	60.633	-3.328	1.00	24.76
4365	N	LEU A	305		67.591	59.677	-1.828	1.00	25.18
4367	CA	LEU A	305		67.117	60.499	-0.711	1.00	25.23
4369	CB	LEU A	305		67.707	59.988	0.608	1.00	25.28
4372	CG	LEU A	305		67.209	60.548	1.945	1.00	27.23
4374	CD1	LEU A	305		67.788	61.919	2.199	1.00	29.43
4378	CD2	LEU A	305		65.687	60.595	2.012	1.00	28.69
4382	C	LEU A	305		67.520	61.954	-0.959	1.00	24.32
4383	O	LEU A	305		66.719	62.872	-0.780	1.00	23.70
4384	N	ALA A	306		68.758	62.146	-1.399	1.00	23.80
4386	CA	ALA A	306		69.282	63.481	-1.672	1.00	24.14
4388	CB	ALA A	306		70.733	63.405	-2.153	1.00	24.17
4392	C	ALA A	306		68.410	64.218	-2.687	1.00	24.07
4393	O	ALA A	306		68.063	65.382	-2.480	1.00	23.69
4394	N	ASP A	307		68.027	63.538	-3.761	1.00	24.24
4396	CA	ASP A	307		67.146	64.143	-4.772	1.00	24.99
4398	CB	ASP A	307		67.015	63.231	-5.990	1.00	25.46
4401	CG	ASP A	307		68.259	63.225	-6.840	1.00	27.73
4402	OD1	ASP A	307		68.311	62.445	-7.819	1.00	32.11
4403	OD2	ASP A	307		69.231	63.968	-6.614	1.00	30.06
4404	C	ASP A	307		65.751	64.427	-4.242	1.00	24.15
4405	O	ASP A	307		65.146	65.464	-4.565	1.00	23.53
4406	N	TYR A	308		65.233	63.497	-3.445	1.00	23.64
4408	CA	TYR A	308		63.890	63.636	-2.889	1.00	23.49
4410	CB	TYR A	308		63.465	62.369	-2.150	1.00	23.53
4413	CG	TYR A	308		62.066	62.432	-1.543	1.00	23.83
4414	CD1	TYR A	308		61.882	62.358	-0.171	1.00	24.83
4416	CE1	TYR A	308		60.607	62.425	0.392	1.00	25.12
4418	CZ	TYR A	308		59.501	62.553	-0.424	1.00	26.00
4419	OH	TYR A	308		58.239	62.602	0.134	1.00	26.70
4421	CE2	TYR A	308		59.660	62.622	-1.798	1.00	25.30
4423	CD2	TYR A	308		60.939	62.568	-2.344	1.00	23.99
4425	C	TYR A	308		63.824	64.844	-1.957	1.00	23.57
4426	O	TYR A	308		62.829	65.529	-1.919	1.00	22.72
4427	N	ILE A	309		64.902	65.112	-1.229	1.00	24.12
4429	CA	ILE A	309		64.949	66.247	-0.301	1.00	24.93
4431	CB	ILE A	309		66.333	66.304	0.411	1.00	24.90
4433	CG1	ILE A	309		66.333	65.285	1.553	1.00	25.34
4436	CD1	ILE A	309		67.675	65.077	2.197	1.00	27.41
4440	CG2	ILE A	309		66.639	67.710	0.943	1.00	25.11
4444	C	ILE A	309		64.575	67.576	-0.977	1.00	25.41
4445	O	ILE A	309		64.017	68.468	-0.326	1.00	25.21
4446	N	ILE A	310		64.848	67.702	-2.274	1.00	25.98
4448	CA	ILE A	310		64.481	68.928	-3.003	1.00	26.46
4450	CB	ILE A	310		65.736	69.586	-3.590	1.00	26.50
4452	CG1	ILE A	310		66.349	68.722	-4.700	1.00	26.76
4455	CD1	ILE A	310		67.350	69.472	-5.530	1.00	27.27
4459	CG2	ILE A	310		66.729	69.819	-2.491	1.00	26.11
4463	C	ILE A	310		63.393	68.781	-4.066	1.00	26.91
4464	O	ILE A	310		62.930	69.779	-4.622	1.00	26.80
4465	N	GLN A	311		62.982	67.543	-4.337	1.00	26.94
4467	CA	GLN A	311		61.911	67.267	-5.284	1.00	27.25

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4469	CB	GLN	A	311	62.217	65.999	-6.089	1.00	27.44
4472	CG	GLN	A	311	63.241	66.219	-7.186	1.00	30.05
4475	CD	GLN	A	311	63.720	64.922	-7.830	1.00	33.37
4476	OE1	GLN	A	311	64.730	64.920	-8.521	1.00	36.33
4477	NE2	GLN	A	311	62.999	63.828	-7.606	1.00	34.01
4480	C	GLN	A	311	60.573	67.102	-4.575	1.00	26.71
4481	O	GLN	A	311	59.514	67.225	-5.193	1.00	27.01
4482	N	ARG	A	312	60.620	66.825	-3.280	1.00	26.09
4484	CA	ARG	A	312	59.418	66.570	-2.503	1.00	25.94
4486	CB	ARG	A	312	59.774	66.077	-1.098	1.00	25.87
4489	CG	ARG	A	312	60.382	67.160	-0.225	1.00	25.06
4492	CD	ARG	A	312	61.211	66.630	0.914	1.00	23.99
4495	NE	ARG	A	312	61.963	67.704	1.555	1.00	22.64
4497	CZ	ARG	A	312	61.503	68.481	2.528	1.00	19.61
4498	NH1	ARG	A	312	62.286	69.429	3.025	1.00	20.15
4501	NH2	ARG	A	312	60.289	68.325	3.008	1.00	19.15
4504	C	ARG	A	312	58.558	67.817	-2.386	1.00	26.24
4505	O	ARG	A	312	59.053	68.938	-2.448	1.00	25.48
4506	N	ASN	A	313	57.269	67.601	-2.191	1.00	26.97
4508	CA	ASN	A	313	56.321	68.702	-2.054	1.00	28.44
4510	CB	ASN	A	313	55.255	68.594	-3.128	1.00	28.90
4513	CG	ASN	A	313	55.820	68.829	-4.487	1.00	31.25
4514	OD1	ASN	A	313	56.328	69.921	-4.771	1.00	36.72
4515	ND2	ASN	A	313	55.782	67.807	-5.337	1.00	35.16
4518	C	ASN	A	313	55.711	68.729	-0.676	1.00	28.47
4519	O	ASN	A	313	54.731	69.426	-0.440	1.00	28.00
4520	N	LYS	A	314	56.326	67.972	0.234	1.00	29.44
4522	CA	LYS	A	314	55.925	67.944	1.642	1.00	30.19
4524	CB	LYS	A	314	54.722	67.029	1.835	1.00	30.27
4527	CG	LYS	A	314	54.874	65.638	1.202	1.00	32.14
4530	CD	LYS	A	314	54.635	64.498	2.180	1.00	34.17
4533	CE	LYS	A	314	53.660	63.459	1.652	1.00	35.54
4536	NZ	LYS	A	314	54.228	62.656	0.542	1.00	36.19
4540	C	LYS	A	314	57.081	67.487	2.528	1.00	30.38
4541	O	LYS	A	314	56.992	67.504	3.759	1.00	30.94
4542	OXT	LYS	A	314	58.130	67.081	2.028	1.00	30.00
4543	N	ASP	B	17	19.060	6.498	-16.010	1.00	36.37
4545	CA	ASP	B	17	17.827	7.340	-15.968	1.00	36.07
4547	CB	ASP	B	17	16.585	6.454	-15.910	1.00	36.75
4550	CG	ASP	B	17	15.301	7.258	-15.889	1.00	38.21
4551	OD1	ASP	B	17	15.288	8.356	-16.476	1.00	42.09
4552	OD2	ASP	B	17	14.258	6.882	-15.321	1.00	41.73
4553	C	ASP	B	17	17.853	8.266	-14.742	1.00	35.62
4554	O	ASP	B	17	17.713	7.800	-13.603	1.00	35.09
4557	N	PHE	B	18	18.002	9.572	-14.969	1.00	34.42
4559	CA	PHE	B	18	18.233	10.472	-13.845	1.00	33.65
4561	CB	PHE	B	18	18.831	11.812	-14.264	1.00	33.54
4564	CG	PHE	B	18	19.286	12.629	-13.097	1.00	32.06
4565	CD1	PHE	B	18	20.342	12.202	-12.312	1.00	31.59
4567	CE1	PHE	B	18	20.747	12.940	-11.217	1.00	31.53
4569	CZ	PHE	B	18	20.080	14.100	-10.888	1.00	30.24
4571	CE2	PHE	B	18	19.029	14.516	-11.638	1.00	31.16

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4573	CD2	PHE	B	18	18.621	13.779	-12.739	1.00	32.52
4575	C	PHE	B	18	17.015	10.695	-12.946	1.00	33.05
4576	O	PHE	B	18	17.179	10.672	-11.738	1.00	32.55
4577	N	PRO	B	19	15.817	10.901	-13.503	1.00	32.85
4578	CA	PRO	B	19	14.606	11.056	-12.680	1.00	32.66
4580	CB	PRO	B	19	13.497	11.261	-13.722	1.00	32.79
4583	CG	PRO	B	19	14.213	11.795	-14.914	1.00	33.05
4586	CD	PRO	B	19	15.508	11.051	-14.936	1.00	32.96
4589	C	PRO	B	19	14.285	9.869	-11.768	1.00	32.36
4590	O	PRO	B	19	13.759	10.093	-10.685	1.00	31.80
4591	N	GLN	B	20	14.594	8.643	-12.190	1.00	31.98
4593	CA	GLN	B	20	14.399	7.478	-11.329	1.00	32.12
4595	CB	GLN	B	20	14.282	6.175	-12.145	1.00	32.62
4598	CG	GLN	B	20	12.872	5.922	-12.758	1.00	35.79
4601	CD	GLN	B	20	11.784	5.507	-11.736	1.00	38.90
4602	OE1	GLN	B	20	11.382	4.327	-11.677	1.00	40.51
4603	NE2	GLN	B	20	11.292	6.479	-10.956	1.00	40.37
4606	C	GLN	B	20	15.524	7.368	-10.279	1.00	30.90
4607	O	GLN	B	20	15.304	6.829	-9.213	1.00	30.46
4608	N	GLN	B	21	16.715	7.872	-10.583	1.00	30.18
4610	CA	GLN	B	21	17.778	7.963	-9.575	1.00	30.30
4612	CB	GLN	B	21	19.108	8.421	-10.180	1.00	30.56
4615	CG	GLN	B	21	19.929	7.310	-10.799	1.00	33.30
4618	CD	GLN	B	21	20.971	6.745	-9.843	1.00	36.37
4619	OE1	GLN	B	21	21.903	7.457	-9.441	1.00	39.14
4620	NE2	GLN	B	21	20.822	5.474	-9.479	1.00	36.91
4623	C	GLN	B	21	17.364	8.924	-8.464	1.00	29.14
4624	O	GLN	B	21	17.509	8.604	-7.285	1.00	29.47
4625	N	LEU	B	22	16.838	10.086	-8.841	1.00	27.84
4627	CA	LEU	B	22	16.384	11.074	-7.864	1.00	27.57
4629	CB	LEU	B	22	15.793	12.309	-8.546	1.00	27.88
4632	CG	LEU	B	22	16.740	13.324	-9.180	1.00	28.18
4634	CD1	LEU	B	22	15.884	14.370	-9.884	1.00	28.62
4638	CD2	LEU	B	22	17.667	13.973	-8.145	1.00	28.38
4642	C	LEU	B	22	15.317	10.478	-6.961	1.00	27.38
4643	O	LEU	B	22	15.364	10.643	-5.741	1.00	26.09
4644	N	GLU	B	23	14.358	9.786	-7.573	1.00	27.02
4646	CA	GLU	B	23	13.207	9.269	-6.847	1.00	27.65
4648	CB	GLU	B	23	12.098	8.855	-7.825	1.00	28.49
4651	CG	GLU	B	23	11.022	7.981	-7.212	1.00	32.02
4654	CD	GLU	B	23	9.646	8.256	-7.782	1.00	37.15
4655	OE1	GLU	B	23	9.109	9.364	-7.545	1.00	42.58
4656	OE2	GLU	B	23	9.100	7.363	-8.463	1.00	41.15
4657	C	GLU	B	23	13.618	8.112	-5.938	1.00	26.50
4658	O	GLU	B	23	13.115	8.008	-4.823	1.00	26.62
4659	N	ALA	B	24	14.513	7.250	-6.421	1.00	25.43
4661	CA	ALA	B	24	15.092	6.179	-5.610	1.00	24.85
4663	CB	ALA	B	24	16.021	5.297	-6.443	1.00	24.98
4667	C	ALA	B	24	15.864	6.765	-4.421	1.00	24.65
4668	O	ALA	B	24	15.827	6.211	-3.318	1.00	23.25
4669	N	CYS	B	25	16.556	7.885	-4.650	1.00	24.00
4671	CA	CYS	B	25	17.315	8.544	-3.589	1.00	23.64

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4673	CB	CYS	B	25	18.217	9.650	-4.152	1.00	23.72
4676	SG	CYS	B	25	19.117	10.582	-2.885	1.00	22.22
4677	C	CYS	B	25	16.374	9.096	-2.524	1.00	23.27
4678	O	CYS	B	25	16.578	8.876	-1.336	1.00	23.22
4679	N	VAL	B	26	15.323	9.779	-2.945	1.00	23.25
4681	CA	VAL	B	26	14.334	10.280	-2.006	1.00	23.43
4683	CB	VAL	B	26	13.175	10.997	-2.725	1.00	23.51
4685	CG1	VAL	B	26	12.005	11.220	-1.804	1.00	24.68
4689	CG2	VAL	B	26	13.650	12.324	-3.276	1.00	23.07
4693	C	VAL	B	26	13.811	9.132	-1.138	1.00	23.73
4694	O	VAL	B	26	13.641	9.300	0.067	1.00	23.38
4695	N	LYS	B	27	13.581	7.964	-1.737	1.00	23.54
4697	CA	LYS	B	27	13.012	6.852	-0.972	1.00	24.03
4699	CB	LYS	B	27	12.440	5.765	-1.891	1.00	24.27
4702	CG	LYS	B	27	10.995	6.086	-2.256	1.00	27.21
4705	CD	LYS	B	27	10.544	5.567	-3.606	1.00	31.82
4708	CE	LYS	B	27	9.032	5.811	-3.762	1.00	33.94
4711	NZ	LYS	B	27	8.488	5.279	-5.045	1.00	37.62
4715	C	LYS	B	27	14.026	6.287	-0.004	1.00	22.89
4716	O	LYS	B	27	13.699	6.017	1.145	1.00	23.39
4717	N	GLN	B	28	15.257	6.124	-0.468	1.00	22.27
4719	CA	GLN	B	28	16.335	5.645	0.380	1.00	21.89
4721	CB	GLN	B	28	17.623	5.496	-0.423	1.00	21.61
4724	CG	GLN	B	28	18.810	4.946	0.352	1.00	21.80
4727	CD	GLN	B	28	18.683	3.471	0.705	1.00	23.69
4728	OE1	GLN	B	28	19.316	2.999	1.657	1.00	25.82
4729	NE2	GLN	B	28	17.882	2.742	-0.054	1.00	22.57
4732	C	GLN	B	28	16.518	6.604	1.561	1.00	21.61
4733	O	GLN	B	28	16.596	6.163	2.704	1.00	21.00
4734	N	ALA	B	29	16.556	7.906	1.285	1.00	21.58
4736	CA	ALA	B	29	16.835	8.916	2.323	1.00	21.82
4738	CB	ALA	B	29	17.120	10.295	1.691	1.00	21.91
4742	C	ALA	B	29	15.684	9.025	3.317	1.00	21.73
4743	O	ALA	B	29	15.897	9.174	4.508	1.00	21.94
4744	N	ASN	B	30	14.461	8.963	2.822	1.00	22.10
4746	CA	ASN	B	30	13.289	8.996	3.699	1.00	22.38
4748	CB	ASN	B	30	12.013	9.035	2.869	1.00	22.05
4751	CG	ASN	B	30	11.720	10.416	2.319	1.00	23.08
4752	OD1	ASN	B	30	12.374	11.387	2.689	1.00	22.74
4753	ND2	ASN	B	30	10.732	10.510	1.424	1.00	22.09
4756	C	ASN	B	30	13.237	7.812	4.655	1.00	22.64
4757	O	ASN	B	30	12.857	7.962	5.811	1.00	22.97
4758	N	GLN	B	31	13.604	6.637	4.160	1.00	22.84
4760	CA	GLN	B	31	13.624	5.438	4.978	1.00	23.34
4762	CB	GLN	B	31	13.859	4.210	4.085	1.00	23.43
4765	CG	GLN	B	31	14.118	2.893	4.795	1.00	26.33
4768	CD	GLN	B	31	14.528	1.795	3.815	1.00	28.80
4769	OE1	GLN	B	31	15.700	1.679	3.443	1.00	33.07
4770	NE2	GLN	B	31	13.560	1.007	3.378	1.00	32.12
4773	C	GLN	B	31	14.720	5.582	6.039	1.00	23.12
4774	O	GLN	B	31	14.542	5.183	7.178	1.00	23.43
4775	N	ALA	B	32	15.855	6.146	5.653	1.00	22.32

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4777	CA	ALA	B	32	16.974	6.318	6.569	1.00	22.90
4779	CB	ALA	B	32	18.199	6.814	5.818	1.00	22.55
4783	C	ALA	B	32	16.590	7.296	7.679	1.00	22.66
4784	O	ALA	B	32	16.750	6.992	8.861	1.00	22.59
4785	N	LEU	B	33	16.069	8.457	7.288	1.00	22.88
4787	CA	LEU	B	33	15.603	9.462	8.244	1.00	23.19
4789	CB	LEU	B	33	14.980	10.661	7.521	1.00	23.23
4792	CG	LEU	B	33	15.948	11.654	6.869	1.00	24.18
4794	CD1	LEU	B	33	15.253	12.531	5.850	1.00	25.04
4798	CD2	LEU	B	33	16.610	12.528	7.925	1.00	25.95
4802	C	LEU	B	33	14.565	8.869	9.206	1.00	23.67
4803	O	LEU	B	33	14.665	9.037	10.415	1.00	22.94
4804	N	SER	B	34	13.573	8.180	8.654	1.00	24.43
4806	CA	SER	B	34	12.506	7.580	9.458	1.00	25.35
4808	CB	SER	B	34	11.490	6.887	8.551	1.00	25.51
4811	OG	SER	B	34	10.877	7.830	7.706	1.00	26.80
4813	C	SER	B	34	13.043	6.579	10.487	1.00	25.98
4814	O	SER	B	34	12.547	6.525	11.610	1.00	26.04
4815	N	ARG	B	35	14.062	5.813	10.094	1.00	26.60
4817	CA	ARG	B	35	14.700	4.820	10.962	1.00	27.70
4819	CB	ARG	B	35	15.743	3.993	10.185	1.00	28.27
4822	CG	ARG	B	35	15.205	2.761	9.484	1.00	31.67
4825	CD	ARG	B	35	16.207	1.605	9.357	1.00	34.70
4828	NE	ARG	B	35	17.593	2.056	9.140	1.00	36.06
4830	CZ	ARG	B	35	18.083	2.498	7.984	1.00	33.83
4831	NH1	ARG	B	35	17.320	2.570	6.914	1.00	34.48
4834	NH2	ARG	B	35	19.354	2.876	7.903	1.00	33.58
4837	C	ARG	B	35	15.407	5.464	12.148	1.00	27.46
4838	O	ARG	B	35	15.465	4.877	13.237	1.00	27.43
4839	N	PHE	B	36	15.967	6.655	11.926	1.00	27.31
4841	CA	PHE	B	36	16.692	7.373	12.965	1.00	26.91
4843	CB	PHE	B	36	17.758	8.289	12.356	1.00	26.72
4846	CG	PHE	B	36	18.835	7.547	11.623	1.00	24.89
4847	CD1	PHE	B	36	19.206	7.916	10.343	1.00	22.57
4849	CE1	PHE	B	36	20.201	7.220	9.656	1.00	22.79
4851	CZ	PHE	B	36	20.845	6.150	10.267	1.00	23.00
4853	CE2	PHE	B	36	20.493	5.777	11.546	1.00	24.18
4855	CD2	PHE	B	36	19.488	6.473	12.224	1.00	24.53
4857	C	PHE	B	36	15.763	8.164	13.851	1.00	27.56
4858	O	PHE	B	36	16.136	8.505	14.964	1.00	28.14
4859	N	ILE	B	37	14.563	8.457	13.357	1.00	28.06
4861	CA	ILE	B	37	13.570	9.208	14.113	1.00	29.01
4863	CB	ILE	B	37	12.677	10.054	13.160	1.00	29.24
4865	CG1	ILE	B	37	13.470	11.240	12.608	1.00	28.43
4868	CD1	ILE	B	37	12.767	12.003	11.524	1.00	29.06
4872	CG2	ILE	B	37	11.412	10.552	13.876	1.00	30.14
4876	C	ILE	B	37	12.719	8.257	14.959	1.00	29.75
4877	O	ILE	B	37	12.120	8.678	15.948	1.00	30.10
4878	N	ALA	B	38	12.698	6.977	14.580	1.00	30.36
4880	CA	ALA	B	38	11.784	5.995	15.172	1.00	30.63
4882	CB	ALA	B	38	11.849	4.666	14.409	1.00	30.80
4886	C	ALA	B	38	12.021	5.762	16.651	1.00	30.90

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4887	O	ALA	B	38	11.052	5.739	17.415	1.00	31.31
4888	N	PRO	B	39	13.278	5.595	17.074	1.00	31.28
4889	CA	PRO	B	39	13.573	5.370	18.494	1.00	31.54
4891	CB	PRO	B	39	15.045	4.922	18.489	1.00	31.77
4894	CG	PRO	B	39	15.425	4.741	17.062	1.00	32.00
4897	CD	PRO	B	39	14.512	5.594	16.270	1.00	31.28
4900	C	PRO	B	39	13.423	6.610	19.377	1.00	31.62
4901	O	PRO	B	39	13.551	6.466	20.594	1.00	32.39
4902	N	LEU	B	40	13.184	7.790	18.794	1.00	30.70
4904	CA	LEU	B	40	13.053	9.012	19.575	1.00	30.07
4906	CB	LEU	B	40	12.980	10.253	18.670	1.00	30.11
4909	CG	LEU	B	40	14.228	10.593	17.836	1.00	30.37
4911	CD1	LEU	B	40	13.985	11.886	17.056	1.00	30.25
4915	CD2	LEU	B	40	15.502	10.691	18.687	1.00	30.52
4919	C	LEU	B	40	11.801	8.963	20.448	1.00	29.37
4920	O	LEU	B	40	10.747	8.494	20.005	1.00	29.73
4921	N	PRO	B	41	11.903	9.477	21.669	1.00	28.40
4922	CA	PRO	B	41	10.738	9.551	22.553	1.00	28.09
4924	CB	PRO	B	41	11.355	9.872	23.921	1.00	28.24
4927	CG	PRO	B	41	12.658	10.565	23.613	1.00	28.08
4930	CD	PRO	B	41	13.115	10.033	22.301	1.00	28.09
4933	C	PRO	B	41	9.796	10.657	22.100	1.00	27.75
4934	O	PRO	B	41	10.119	11.411	21.154	1.00	26.90
4935	N	PHE	B	42	8.630	10.724	22.739	1.00	27.16
4937	CA	PHE	B	42	7.644	11.774	22.477	1.00	27.19
4939	CB	PHE	B	42	8.224	13.158	22.776	1.00	27.06
4942	CG	PHE	B	42	8.887	13.259	24.118	1.00	27.64
4943	CD1	PHE	B	42	8.136	13.124	25.279	1.00	28.66
4945	CE1	PHE	B	42	8.732	13.207	26.518	1.00	29.45
4947	CZ	PHE	B	42	10.096	13.439	26.617	1.00	28.49
4949	CE2	PHE	B	42	10.863	13.574	25.475	1.00	27.66
4951	CD2	PHE	B	42	10.260	13.485	24.226	1.00	27.57
4953	C	PHE	B	42	7.094	11.730	21.053	1.00	27.15
4954	O	PHE	B	42	6.729	12.755	20.491	1.00	26.43
4955	N	GLN	B	43	7.015	10.534	20.489	1.00	27.91
4957	CA	GLN	B	43	6.310	10.320	19.224	1.00	28.60
4959	CB	GLN	B	43	6.294	8.834	18.858	1.00	28.40
4962	CG	GLN	B	43	7.659	8.201	18.665	1.00	28.70
4965	CD	GLN	B	43	8.379	8.718	17.438	1.00	28.74
4966	OE1	GLN	B	43	7.765	8.927	16.394	1.00	29.53
4967	NE2	GLN	B	43	9.685	8.915	17.558	1.00	28.45
4970	C	GLN	B	43	4.868	10.796	19.363	1.00	29.43
4971	O	GLN	B	43	4.275	10.720	20.449	1.00	30.02
4972	N	ASN	B	44	4.311	11.291	18.268	1.00	30.07
4974	CA	ASN	B	44	2.942	11.787	18.226	1.00	30.82
4976	CB	ASN	B	44	1.943	10.631	18.396	1.00	31.34
4979	CG	ASN	B	44	2.264	9.445	17.492	1.00	32.36
4980	OD1	ASN	B	44	2.338	9.579	16.261	1.00	35.83
4981	ND2	ASN	B	44	2.480	8.288	18.096	1.00	33.67
4984	C	ASN	B	44	2.684	12.898	19.244	1.00	30.94
4985	O	ASN	B	44	1.596	12.983	19.805	1.00	31.98
4986	N	THR	B	45	3.705	13.716	19.507	1.00	30.13

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4988	CA	THR	B	45	3.529	14.982	20.201	1.00	29.44
4990	CB	THR	B	45	4.399	15.055	21.470	1.00	29.55
4992	OG1	THR	B	45	5.790	15.106	21.123	1.00	29.59
4994	CG2	THR	B	45	4.249	13.787	22.313	1.00	30.13
4998	C	THR	B	45	3.901	16.083	19.216	1.00	28.76
4999	O	THR	B	45	4.574	15.800	18.231	1.00	29.08
5000	N	PRO	B	46	3.458	17.318	19.450	1.00	28.09
5001	CA	PRO	B	46	3.684	18.421	18.494	1.00	27.28
5003	CB	PRO	B	46	3.174	19.652	19.252	1.00	27.82
5006	CG	PRO	B	46	2.115	19.111	20.181	1.00	28.40
5009	CD	PRO	B	46	2.640	17.750	20.605	1.00	28.19
5012	C	PRO	B	46	5.135	18.643	18.041	1.00	26.19
5013	O	PRO	B	46	5.357	18.854	16.853	1.00	25.60
5014	N	VAL	B	47	6.100	18.595	18.957	1.00	24.76
5016	CA	VAL	B	47	7.479	18.902	18.602	1.00	23.94
5018	CB	VAL	B	47	8.365	19.173	19.859	1.00	24.25
5020	CG1	VAL	B	47	8.593	17.904	20.684	1.00	24.46
5024	CG2	VAL	B	47	9.678	19.801	19.452	1.00	25.37
5028	C	VAL	B	47	8.074	17.824	17.690	1.00	22.86
5029	O	VAL	B	47	8.719	18.150	16.704	1.00	21.98
5030	N	VAL	B	48	7.822	16.549	17.991	1.00	22.17
5032	CA	VAL	B	48	8.303	15.456	17.145	1.00	22.05
5034	CB	VAL	B	48	8.227	14.101	17.872	1.00	22.22
5036	CG1	VAL	B	48	8.620	12.960	16.951	1.00	22.38
5040	CG2	VAL	B	48	9.132	14.128	19.090	1.00	22.62
5044	C	VAL	B	48	7.547	15.414	15.816	1.00	22.15
5045	O	VAL	B	48	8.108	15.076	14.775	1.00	21.53
5046	N	GLU	B	49	6.273	15.760	15.844	1.00	22.30
5048	CA	GLU	B	49	5.501	15.839	14.612	1.00	23.31
5050	CB	GLU	B	49	4.020	16.062	14.906	1.00	23.97
5053	CG	GLU	B	49	3.349	14.847	15.529	1.00	27.97
5056	CD	GLU	B	49	1.902	15.107	15.899	1.00	32.93
5057	OE1	GLU	B	49	1.410	16.237	15.650	1.00	37.74
5058	OE2	GLU	B	49	1.263	14.182	16.446	1.00	36.88
5059	C	GLU	B	49	6.023	16.965	13.727	1.00	22.40
5060	O	GLU	B	49	6.016	16.837	12.516	1.00	21.26
5061	N	THR	B	50	6.497	18.044	14.344	1.00	21.39
5063	CA	THR	B	50	7.105	19.143	13.607	1.00	21.78
5065	CB	THR	B	50	7.382	20.353	14.534	1.00	22.24
5067	OG1	THR	B	50	6.174	20.767	15.191	1.00	21.33
5069	CG2	THR	B	50	7.803	21.573	13.727	1.00	22.96
5073	C	THR	B	50	8.406	18.684	12.964	1.00	21.83
5074	O	THR	B	50	8.671	19.001	11.808	1.00	21.23
5075	N	MET	B	51	9.220	17.953	13.728	1.00	21.95
5077	CA	MET	B	51	10.470	17.408	13.215	1.00	21.91
5079	CB	MET	B	51	11.207	16.630	14.299	1.00	21.87
5082	CG	MET	B	51	11.735	17.485	15.441	1.00	20.93
5085	SD	MET	B	51	12.315	16.444	16.774	1.00	22.35
5086	CE	MET	B	51	13.754	15.689	16.047	1.00	23.07
5090	C	MET	B	51	10.221	16.502	12.014	1.00	22.56
5091	O	MET	B	51	10.951	16.565	11.024	1.00	22.83
5092	N	GLN	B	52	9.179	15.676	12.088	1.00	23.09

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5094	CA	GLN	B	52	8.895	14.714	11.016	1.00	23.09
5096	CB	GLN	B	52	7.843	13.694	11.460	1.00	23.18
5099	CG	GLN	B	52	8.386	12.700	12.456	1.00	24.11
5102	CD	GLN	B	52	7.334	11.743	12.961	1.00	26.66
5103	OE1	GLN	B	52	7.463	10.525	12.791	1.00	28.62
5104	NE2	GLN	B	52	6.304	12.280	13.601	1.00	23.91
5107	C	GLN	B	52	8.393	15.435	9.787	1.00	22.65
5108	O	GLN	B	52	8.764	15.123	8.661	1.00	22.15
5109	N	TYR	B	53	7.531	16.402	10.028	1.00	22.64
5111	CA	TYR	B	53	6.942	17.213	8.974	1.00	22.81
5113	CB	TYR	B	53	5.939	18.145	9.647	1.00	23.23
5116	CG	TYR	B	53	5.133	19.066	8.784	1.00	24.77
5117	CD1	TYR	B	53	3.855	18.706	8.346	1.00	27.29
5119	CE1	TYR	B	53	3.089	19.572	7.587	1.00	28.69
5121	CZ	TYR	B	53	3.582	20.820	7.286	1.00	28.49
5122	OH	TYR	B	53	2.827	21.673	6.537	1.00	28.74
5124	CE2	TYR	B	53	4.844	21.209	7.727	1.00	27.93
5126	CD2	TYR	B	53	5.600	20.335	8.477	1.00	26.79
5128	C	TYR	B	53	8.051	17.978	8.237	1.00	22.85
5129	O	TYR	B	53	8.114	17.976	7.010	1.00	22.68
5130	N	GLY	B	54	8.948	18.591	9.005	1.00	22.75
5132	CA	GLY	B	54	10.014	19.408	8.455	1.00	22.25
5135	C	GLY	B	54	11.071	18.608	7.738	1.00	22.08
5136	O	GLY	B	54	11.669	19.088	6.782	1.00	21.36
5137	N	ALA	B	55	11.310	17.384	8.201	1.00	22.33
5139	CA	ALA	B	55	12.382	16.568	7.656	1.00	22.52
5141	CB	ALA	B	55	12.996	15.714	8.733	1.00	22.31
5145	C	ALA	B	55	11.925	15.698	6.492	1.00	23.07
5146	O	ALA	B	55	12.692	15.487	5.548	1.00	22.77
5147	N	LEU	B	56	10.682	15.220	6.538	1.00	23.33
5149	CA	LEU	B	56	10.265	14.079	5.705	1.00	24.30
5151	CB	LEU	B	56	9.706	12.960	6.586	1.00	24.12
5154	CG	LEU	B	56	10.789	12.220	7.367	1.00	24.95
5156	CD1	LEU	B	56	10.177	11.362	8.448	1.00	25.81
5160	CD2	LEU	B	56	11.624	11.386	6.415	1.00	25.72
5164	C	LEU	B	56	9.241	14.390	4.610	1.00	24.83
5165	O	LEU	B	56	9.168	13.668	3.615	1.00	24.82
5166	N	LEU	B	57	8.480	15.459	4.784	1.00	25.44
5168	CA	LEU	B	57	7.363	15.761	3.890	1.00	26.38
5170	CB	LEU	B	57	6.196	16.353	4.683	1.00	26.51
5173	CG	LEU	B	57	4.851	15.625	4.607	1.00	29.53
5175	CD1	LEU	B	57	4.953	14.108	4.807	1.00	30.58
5179	CD2	LEU	B	57	3.880	16.228	5.625	1.00	30.77
5183	C	LEU	B	57	7.833	16.671	2.741	1.00	26.06
5184	O	LEU	B	57	7.862	17.895	2.846	1.00	27.01
5185	N	GLY	B	58	8.237	16.048	1.651	1.00	25.60
5187	CA	GLY	B	58	8.677	16.778	0.477	1.00	25.47
5190	C	GLY	B	58	10.152	17.095	0.529	1.00	24.67
5191	O	GLY	B	58	10.821	16.878	1.542	1.00	24.85
5192	N	GLY	B	59	10.655	17.628	-0.575	1.00	24.17
5194	CA	GLY	B	59	12.046	18.001	-0.702	1.00	23.50
5197	C	GLY	B	59	12.688	17.037	-1.671	1.00	23.34

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5198	O	GLY	B	59	12.221	15.901	-1.822	1.00	23.79
5199	N	LYS	B	60	13.776	17.465	-2.305	1.00	22.25
5201	CA	LYS	B	60	14.378	16.698	-3.397	1.00	21.47
5203	CB	LYS	B	60	14.964	17.634	-4.446	1.00	21.33
5206	CG	LYS	B	60	13.989	18.633	-5.009	1.00	21.64
5209	CD	LYS	B	60	14.690	19.563	-5.983	1.00	20.05
5212	CE	LYS	B	60	15.503	20.635	-5.285	1.00	20.61
5215	NZ	LYS	B	60	14.661	21.571	-4.488	1.00	18.47
5219	C	LYS	B	60	15.473	15.764	-2.916	1.00	20.81
5220	O	LYS	B	60	15.930	14.904	-3.680	1.00	19.71
5221	N	ARG	B	61	15.873	15.934	-1.651	1.00	19.67
5223	CA	ARG	B	61	16.956	15.168	-1.037	1.00	19.66
5225	CB	ARG	B	61	16.531	13.713	-0.785	1.00	19.62
5228	CG	ARG	B	61	15.280	13.581	0.031	1.00	20.32
5231	CD	ARG	B	61	15.456	13.814	1.534	1.00	21.36
5234	NE	ARG	B	61	14.145	13.667	2.159	1.00	22.35
5236	CZ	ARG	B	61	13.232	14.625	2.243	1.00	24.57
5237	NH1	ARG	B	61	13.491	15.867	1.836	1.00	25.55
5240	NH2	ARG	B	61	12.042	14.347	2.754	1.00	25.42
5243	C	ARG	B	61	18.218	15.188	-1.878	1.00	19.19
5244	O	ARG	B	61	18.871	14.162	-2.042	1.00	19.59
5245	N	LEU	B	62	18.575	16.345	-2.419	1.00	18.57
5247	CA	LEU	B	62	19.781	16.421	-3.233	1.00	18.09
5249	CB	LEU	B	62	19.801	17.700	-4.043	1.00	18.16
5252	CG	LEU	B	62	18.659	17.854	-5.069	1.00	17.75
5254	CD1	LEU	B	62	18.918	19.010	-5.960	1.00	17.68
5258	CD2	LEU	B	62	18.460	16.582	-5.902	1.00	17.92
5262	C	LEU	B	62	21.050	16.265	-2.398	1.00	18.27
5263	O	LEU	B	62	22.075	15.828	-2.904	1.00	19.36
5264	N	ARG	B	63	20.984	16.589	-1.118	1.00	18.60
5266	CA	ARG	B	63	22.152	16.472	-0.263	1.00	18.77
5268	CB	ARG	B	63	22.052	17.389	0.948	1.00	18.34
5271	CG	ARG	B	63	22.255	18.855	0.557	1.00	18.92
5274	CD	ARG	B	63	21.763	19.861	1.576	1.00	19.63
5277	NE	ARG	B	63	21.626	21.189	0.993	1.00	18.86
5279	CZ	ARG	B	63	20.623	21.574	0.213	1.00	20.23
5280	NH1	ARG	B	63	20.591	22.816	-0.258	1.00	20.75
5283	NH2	ARG	B	63	19.642	20.736	-0.106	1.00	20.23
5286	C	ARG	B	63	22.421	14.999	0.076	1.00	19.10
5287	O	ARG	B	63	23.547	14.561	-0.077	1.00	19.88
5288	N	PRO	B	64	21.423	14.225	0.504	1.00	19.43
5289	CA	PRO	B	64	21.571	12.764	0.495	1.00	19.41
5291	CB	PRO	B	64	20.168	12.271	0.822	1.00	20.11
5294	CG	PRO	B	64	19.619	13.337	1.712	1.00	19.65
5297	CD	PRO	B	64	20.136	14.628	1.091	1.00	19.55
5300	C	PRO	B	64	22.061	12.230	-0.851	1.00	18.78
5301	O	PRO	B	64	22.971	11.411	-0.850	1.00	19.31
5302	N	PHE	B	65	21.512	12.708	-1.965	1.00	18.78
5304	CA	PHE	B	65	21.994	12.301	-3.290	1.00	18.13
5306	CB	PHE	B	65	21.301	13.089	-4.406	1.00	18.17
5309	CG	PHE	B	65	21.440	12.462	-5.768	1.00	19.67
5310	CD1	PHE	B	65	22.618	12.595	-6.496	1.00	21.70

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5312	CE1	PHE	B	65	22.745	12.007	-7.755	1.00	22.62
5314	CZ	PHE	B	65	21.697	11.280	-8.296	1.00	23.33
5316	CE2	PHE	B	65	20.532	11.138	-7.587	1.00	23.93
5318	CD2	PHE	B	65	20.400	11.730	-6.324	1.00	22.20
5320	C	PHE	B	65	23.518	12.444	-3.401	1.00	18.01
5321	O	PHE	B	65	24.194	11.528	-3.851	1.00	17.71
5322	N	LEU	B	66	24.042	13.591	-2.986	1.00	17.36
5324	CA	LEU	B	66	25.470	13.851	-3.011	1.00	17.79
5326	CB	LEU	B	66	25.775	15.297	-2.615	1.00	17.54
5329	CG	LEU	B	66	25.431	16.355	-3.650	1.00	18.09
5331	CD1	LEU	B	66	25.477	17.733	-3.004	1.00	20.27
5335	CD2	LEU	B	66	26.378	16.312	-4.830	1.00	18.85
5339	C	LEU	B	66	26.245	12.913	-2.104	1.00	17.24
5340	O	LEU	B	66	27.325	12.470	-2.464	1.00	17.66
5341	N	VAL	B	67	25.717	12.633	-0.920	1.00	16.80
5343	CA	VAL	B	67	26.388	11.711	-0.011	1.00	16.74
5345	CB	VAL	B	67	25.658	11.640	1.340	1.00	16.98
5347	CG1	VAL	B	67	26.180	10.504	2.196	1.00	16.26
5351	CG2	VAL	B	67	25.754	13.004	2.088	1.00	17.68
5355	C	VAL	B	67	26.465	10.322	-0.656	1.00	16.74
5356	O	VAL	B	67	27.536	9.725	-0.718	1.00	15.63
5357	N	TYR	B	68	25.315	9.830	-1.120	1.00	17.27
5359	CA	TYR	B	68	25.226	8.520	-1.767	1.00	18.14
5361	CB	TYR	B	68	23.790	8.181	-2.162	1.00	18.15
5364	CG	TYR	B	68	22.884	7.903	-1.001	1.00	17.89
5365	CD1	TYR	B	68	23.205	6.940	-0.059	1.00	19.51
5367	CE1	TYR	B	68	22.357	6.678	1.022	1.00	18.10
5369	CZ	TYR	B	68	21.198	7.396	1.155	1.00	18.28
5370	OH	TYR	B	68	20.351	7.135	2.215	1.00	19.90
5372	CE2	TYR	B	68	20.866	8.363	0.221	1.00	18.45
5374	CD2	TYR	B	68	21.699	8.599	-0.846	1.00	18.98
5376	C	TYR	B	68	26.082	8.438	-3.015	1.00	17.83
5377	O	TYR	B	68	26.788	7.478	-3.201	1.00	17.93
5378	N	ALA	B	69	26.031	9.456	-3.868	1.00	18.14
5380	CA	ALA	B	69	26.687	9.377	-5.168	1.00	17.87
5382	CB	ALA	B	69	26.264	10.525	-6.039	1.00	18.36
5386	C	ALA	B	69	28.200	9.387	-4.975	1.00	18.40
5387	O	ALA	B	69	28.960	8.703	-5.696	1.00	18.10
5388	N	THR	B	70	28.639	10.155	-3.985	1.00	18.02
5390	CA	THR	B	70	30.055	10.258	-3.691	1.00	18.66
5392	CB	THR	B	70	30.300	11.424	-2.750	1.00	17.72
5394	OG1	THR	B	70	29.858	12.636	-3.373	1.00	18.73
5396	CG2	THR	B	70	31.801	11.638	-2.534	1.00	19.07
5400	C	THR	B	70	30.634	8.968	-3.097	1.00	19.24
5401	O	THR	B	70	31.644	8.449	-3.592	1.00	19.75
5402	N	GLY	B	71	29.999	8.474	-2.036	1.00	19.50
5404	CA	GLY	B	71	30.432	7.259	-1.389	1.00	20.08
5407	C	GLY	B	71	30.417	6.071	-2.343	1.00	20.27
5408	O	GLY	B	71	31.314	5.231	-2.310	1.00	20.87
5409	N	HIS	B	72	29.379	6.008	-3.169	1.00	20.75
5411	CA	HIS	B	72	29.201	4.952	-4.163	1.00	21.28
5413	CB	HIS	B	72	27.909	5.167	-4.955	1.00	20.79

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5416	CG	HIS	B	72	26.666	4.749	-4.233	1.00	20.15
5417	ND1	HIS	B	72	25.407	4.975	-4.744	1.00	18.98
5419	CE1	HIS	B	72	24.500	4.502	-3.911	1.00	20.13
5421	NE2	HIS	B	72	25.126	3.949	-2.887	1.00	20.74
5423	CD2	HIS	B	72	26.482	4.101	-3.059	1.00	21.64
5425	C	HIS	B	72	30.361	4.878	-5.151	1.00	21.89
5426	O	HIS	B	72	30.692	3.791	-5.606	1.00	21.76
5427	N	MET	B	73	30.960	6.023	-5.493	1.00	22.15
5429	CA	MET	B	73	32.157	6.051	-6.357	1.00	23.42
5431	CB	MET	B	73	32.672	7.481	-6.565	1.00	23.57
5434	CG	MET	B	73	31.804	8.325	-7.471	1.00	24.99
5437	SD	MET	B	73	32.611	9.844	-8.067	1.00	26.07
5438	CE	MET	B	73	33.270	10.463	-6.588	1.00	25.93
5442	C	MET	B	73	33.303	5.200	-5.819	1.00	23.68
5443	O	MET	B	73	34.094	4.657	-6.595	1.00	24.77
5444	N	PHE	B	74	33.405	5.105	-4.502	1.00	23.69
5446	CA	PHE	B	74	34.474	4.342	-3.856	1.00	23.70
5448	CB	PHE	B	74	35.073	5.171	-2.720	1.00	23.12
5451	CG	PHE	B	74	35.419	6.571	-3.134	1.00	23.22
5452	CD1	PHE	B	74	34.539	7.620	-2.887	1.00	22.52
5454	CE1	PHE	B	74	34.842	8.909	-3.297	1.00	21.95
5456	CZ	PHE	B	74	36.029	9.160	-3.967	1.00	23.61
5458	CE2	PHE	B	74	36.910	8.116	-4.230	1.00	22.42
5460	CD2	PHE	B	74	36.604	6.834	-3.818	1.00	23.20
5462	C	PHE	B	74	34.016	2.986	-3.339	1.00	23.73
5463	O	PHE	B	74	34.751	2.309	-2.625	1.00	23.67
5464	N	GLY	B	75	32.791	2.607	-3.686	1.00	23.96
5466	CA	GLY	B	75	32.273	1.287	-3.397	1.00	24.04
5469	C	GLY	B	75	31.674	1.153	-2.023	1.00	23.99
5470	O	GLY	B	75	31.462	0.038	-1.543	1.00	23.68
5471	N	VAL	B	76	31.385	2.278	-1.375	1.00	23.71
5473	CA	VAL	B	76	30.866	2.207	-0.020	1.00	23.08
5475	CB	BVAL	B	76	31.048	3.547	0.736	0.35	22.92
5476	CB	AVAL	B	76	31.192	3.459	0.840	0.65	23.42
5479	CG1BVAL	B	76		30.368	3.508	2.114	0.35	22.09
5480	CG1AVAL	B	76		32.625	3.934	0.590	0.65	23.81
5487	CG2BVAL	B	76		32.527	3.883	0.872	0.35	23.15
5488	CG2AVAL	B	76		30.219	4.544	0.625	0.65	24.67
5495	C	VAL	B	76	29.387	1.847	-0.088	1.00	22.55
5496	O	VAL	B	76	28.660	2.300	-0.965	1.00	21.42
5497	N	SER	B	77	28.987	0.968	0.819	1.00	22.22
5499	CA	SER	B	77	27.645	0.429	0.868	1.00	22.25
5501	CB	SER	B	77	27.539	-0.621	1.979	1.00	22.22
5504	OG	SER	B	77	26.202	-1.078	2.137	1.00	22.42
5506	C	SER	B	77	26.656	1.550	1.108	1.00	22.33
5507	O	SER	B	77	26.919	2.462	1.898	1.00	21.77
5508	N	THR	B	78	25.534	1.480	0.394	1.00	21.99
5510	CA	THR	B	78	24.431	2.400	0.559	1.00	22.06
5512	CB	THR	B	78	23.259	1.990	-0.367	1.00	22.16
5514	OG1	THR	B	78	23.685	2.032	-1.732	1.00	23.21
5516	CG2	THR	B	78	22.126	2.999	-0.303	1.00	22.58
5520	C	THR	B	78	23.949	2.433	1.997	1.00	21.59

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5521	O	THR	B	78	23.618	3.500	2.527	1.00	21.04
5522	N	ASN	B	79	23.897	1.261	2.628	1.00	21.29
5524	CA	ASN	B	79	23.467	1.170	4.022	1.00	21.08
5526	CB	ASN	B	79	23.358	-0.293	4.454	1.00	21.68
5529	CG	ASN	B	79	23.046	-0.442	5.923	1.00	21.92
5530	OD1	ASN	B	79	21.903	-0.297	6.343	1.00	23.33
5531	ND2	ASN	B	79	24.060	-0.747	6.706	1.00	22.60
5534	C	ASN	B	79	24.404	1.930	4.963	1.00	20.60
5535	O	ASN	B	79	23.950	2.532	5.920	1.00	19.95
5536	N	THR	B	80	25.708	1.876	4.708	1.00	20.20
5538	CA	THR	B	80	26.661	2.698	5.453	1.00	20.29
5540	CB	THR	B	80	28.086	2.339	5.017	1.00	20.31
5542	OG1	THR	B	80	28.386	1.014	5.482	1.00	20.98
5544	CG2	THR	B	80	29.139	3.242	5.699	1.00	21.55
5548	C	THR	B	80	26.390	4.199	5.257	1.00	20.17
5549	O	THR	B	80	26.440	4.994	6.218	1.00	20.64
5550	N	LEU	B	81	26.078	4.560	4.013	1.00	19.46
5552	CA	LEU	B	81	25.883	5.947	3.604	1.00	19.22
5554	CB	LEU	B	81	25.952	6.044	2.077	1.00	18.97
5557	CG	LEU	B	81	27.376	5.905	1.533	1.00	19.26
5559	CD1	LEU	B	81	27.370	5.638	0.037	1.00	20.15
5563	CD2	LEU	B	81	28.251	7.121	1.875	1.00	20.46
5567	C	LEU	B	81	24.584	6.574	4.113	1.00	19.19
5568	O	LEU	B	81	24.445	7.794	4.139	1.00	18.91
5569	N	ASP	B	82	23.641	5.746	4.523	1.00	19.51
5571	CA	ASP	B	82	22.393	6.219	5.106	1.00	19.28
5573	CB	ASP	B	82	21.559	5.046	5.616	1.00	19.89
5576	CG	ASP	B	82	20.654	4.406	4.552	1.00	21.00
5577	OD1	ASP	B	82	20.591	4.823	3.365	1.00	21.03
5578	OD2	ASP	B	82	19.938	3.431	4.867	1.00	24.24
5579	C	ASP	B	82	22.645	7.167	6.297	1.00	18.72
5580	O	ASP	B	82	21.924	8.147	6.462	1.00	18.18
5581	N	ALA	B	83	23.639	6.861	7.130	1.00	18.70
5583	CA	ALA	B	83	23.955	7.700	8.290	1.00	19.48
5585	CB	ALA	B	83	25.006	7.061	9.204	1.00	19.64
5589	C	ALA	B	83	24.360	9.113	7.894	1.00	19.16
5590	O	ALA	B	83	23.679	10.049	8.257	1.00	18.92
5591	N	PRO	B	84	25.451	9.305	7.163	1.00	19.56
5592	CA	PRO	B	84	25.781	10.672	6.739	1.00	19.16
5594	CB	PRO	B	84	27.114	10.519	6.004	1.00	19.21
5597	CG	PRO	B	84	27.166	9.070	5.606	1.00	19.67
5600	CD	PRO	B	84	26.446	8.323	6.694	1.00	19.64
5603	C	PRO	B	84	24.692	11.299	5.856	1.00	18.58
5604	O	PRO	B	84	24.509	12.510	5.924	1.00	18.13
5605	N	ALA	B	85	23.975	10.506	5.063	1.00	18.37
5607	CA	ALA	B	85	22.891	11.038	4.225	1.00	18.51
5609	CB	ALA	B	85	22.314	9.952	3.312	1.00	18.83
5613	C	ALA	B	85	21.790	11.644	5.073	1.00	18.64
5614	O	ALA	B	85	21.313	12.749	4.811	1.00	19.06
5615	N	ALA	B	86	21.407	10.928	6.114	1.00	18.40
5617	CA	ALA	B	86	20.360	11.383	7.010	1.00	18.11
5619	CB	ALA	B	86	19.906	10.245	7.903	1.00	18.05

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5623	C	ALA	B	86	20.855	12.566	7.841	1.00	17.48
5624	O	ALA	B	86	20.123	13.505	8.071	1.00	16.95
5625	N	ALA	B	87	22.105	12.525	8.281	1.00	17.41
5627	CA	ALA	B	87	22.630	13.600	9.115	1.00	17.40
5629	CB	ALA	B	87	23.982	13.244	9.638	1.00	17.13
5633	C	ALA	B	87	22.680	14.917	8.335	1.00	17.61
5634	O	ALA	B	87	22.298	15.947	8.858	1.00	17.33
5635	N	VAL	B	88	23.143	14.893	7.091	1.00	18.42
5637	CA	VAL	B	88	23.208	16.146	6.304	1.00	18.96
5639	CB	BVAL	B	88	24.038	16.002	4.993	0.35	18.97
5640	CB	AVAL	B	88	23.983	16.016	4.957	0.65	19.14
5643	CG1BVAL	B	88		23.256	15.295	3.906	0.35	19.73
5644	CG1AVAL	B	88		25.429	15.726	5.214	0.65	19.11
5651	CG2BVAL	B	88		24.517	17.378	4.509	0.35	18.57
5652	CG2AVAL	B	88		23.381	14.977	4.031	0.65	20.34
5659	C	VAL	B	88	21.813	16.685	6.031	1.00	19.05
5660	O	VAL	B	88	21.610	17.902	6.048	1.00	19.83
5661	N	GLU	B	89	20.858	15.786	5.828	1.00	18.96
5663	CA	GLU	B	89	19.479	16.181	5.611	1.00	19.29
5665	CB	GLU	B	89	18.657	15.024	5.045	1.00	19.83
5668	CG	GLU	B	89	17.271	15.429	4.550	1.00	20.18
5671	CD	GLU	B	89	17.276	16.380	3.353	1.00	21.04
5672	OE1	GLU	B	89	16.175	16.831	2.956	1.00	20.80
5673	OE2	GLU	B	89	18.352	16.669	2.784	1.00	22.55
5674	C	GLU	B	89	18.816	16.727	6.868	1.00	19.09
5675	O	GLU	B	89	17.964	17.587	6.761	1.00	18.76
5676	N	CYS	B	90	19.205	16.246	8.053	1.00	19.19
5678	CA	CYS	B	90	18.694	16.808	9.313	1.00	18.68
5680	CB	CYS	B	90	19.186	16.019	10.519	1.00	19.12
5683	SG	CYS	B	90	18.326	14.474	10.771	1.00	22.59
5684	C	CYS	B	90	19.160	18.255	9.485	1.00	17.90
5685	O	CYS	B	90	18.407	19.095	9.978	1.00	17.58
5686	N	ILE	B	91	20.416	18.524	9.129	1.00	16.55
5688	CA	ILE	B	91	20.951	19.877	9.214	1.00	16.20
5690	CB	ILE	B	91	22.468	19.934	8.896	1.00	15.98
5692	CG1	ILE	B	91	23.261	19.204	9.970	1.00	15.40
5695	CD1	ILE	B	91	23.203	19.886	11.342	1.00	17.23
5699	CG2	ILE	B	91	22.941	21.391	8.777	1.00	15.29
5703	C	ILE	B	91	20.200	20.722	8.215	1.00	15.87
5704	O	ILE	B	91	19.770	21.815	8.533	1.00	15.70
5705	N	HIS	B	92	20.067	20.215	6.992	1.00	15.91
5707	CA	HIS	B	92	19.330	20.914	5.957	1.00	16.10
5709	CB	HIS	B	92	19.247	20.072	4.687	1.00	16.66
5712	CG	HIS	B	92	18.572	20.782	3.567	1.00	15.86
5713	ND1	HIS	B	92	17.518	20.240	2.860	1.00	19.53
5715	CE1	HIS	B	92	17.127	21.104	1.941	1.00	17.62
5717	NE2	HIS	B	92	17.871	22.190	2.043	1.00	19.93
5719	CD2	HIS	B	92	18.776	22.017	3.057	1.00	15.34
5721	C	HIS	B	92	17.923	21.259	6.424	1.00	17.04
5722	O	HIS	B	92	17.524	22.425	6.412	1.00	16.67
5723	N	ALA	B	93	17.193	20.243	6.885	1.00	17.19
5725	CA	ALA	B	93	15.809	20.414	7.334	1.00	17.14

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5727	CB	ALA	B	93	15.236	19.074	7.793	1.00	17.69
5731	C	ALA	B	93	15.681	21.456	8.452	1.00	17.97
5732	O	ALA	B	93	14.806	22.325	8.400	1.00	17.24
5733	N	TYR	B	94	16.570	21.389	9.449	1.00	17.80
5735	CA	TYR	B	94	16.550	22.348	10.560	1.00	17.32
5737	CB	TYR	B	94	17.580	21.968	11.647	1.00	18.17
5740	CG	TYR	B	94	18.635	23.015	11.933	1.00	19.38
5741	CD1	TYR	B	94	18.308	24.219	12.556	1.00	22.96
5743	CE1	TYR	B	94	19.290	25.186	12.809	1.00	23.47
5745	CZ	TYR	B	94	20.601	24.932	12.424	1.00	23.58
5746	OH	TYR	B	94	21.596	25.839	12.653	1.00	22.83
5748	CE2	TYR	B	94	20.935	23.736	11.815	1.00	21.94
5750	CD2	TYR	B	94	19.963	22.802	11.571	1.00	20.83
5752	C	TYR	B	94	16.810	23.765	10.042	1.00	16.90
5753	O	TYR	B	94	16.187	24.727	10.489	1.00	16.75
5754	N	SER	B	95	17.730	23.891	9.098	1.00	16.44
5756	CA	SER	B	95	18.097	25.192	8.581	1.00	17.14
5758	CB	SER	B	95	19.263	25.083	7.593	1.00	16.73
5761	OG	SER	B	95	18.840	24.597	6.337	1.00	18.73
5763	C	SER	B	95	16.887	25.851	7.924	1.00	17.47
5764	O	SER	B	95	16.686	27.050	8.047	1.00	17.44
5765	N	LEU	B	96	16.089	25.064	7.224	1.00	18.06
5767	CA	LEU	B	96	14.897	25.584	6.562	1.00	18.72
5769	CB	LEU	B	96	14.324	24.528	5.642	1.00	19.20
5772	CG	LEU	B	96	15.224	23.982	4.548	1.00	19.55
5774	CD1	LEU	B	96	14.392	23.084	3.642	1.00	21.29
5778	CD2	LEU	B	96	15.912	25.114	3.771	1.00	19.66
5782	C	LEU	B	96	13.814	26.018	7.551	1.00	18.78
5783	O	LEU	B	96	13.179	27.057	7.360	1.00	19.38
5784	N	ILE	B	97	13.607	25.227	8.599	1.00	18.35
5786	CA	ILE	B	97	12.581	25.536	9.612	1.00	18.39
5788	CB	ILE	B	97	12.525	24.456	10.724	1.00	18.49
5790	CG1	ILE	B	97	12.050	23.122	10.161	1.00	19.38
5793	CD1	ILE	B	97	12.339	21.950	11.075	1.00	20.40
5797	CG2	ILE	B	97	11.617	24.887	11.862	1.00	18.22
5801	C	ILE	B	97	12.874	26.891	10.247	1.00	18.35
5802	O	ILE	B	97	11.976	27.698	10.437	1.00	18.38
5803	N	HIS	B	98	14.142	27.127	10.568	1.00	18.85
5805	CA	HIS	B	98	14.554	28.377	11.204	1.00	18.52
5807	CB	HIS	B	98	15.891	28.199	11.898	1.00	19.08
5810	CG	HIS	B	98	15.787	27.494	13.204	1.00	18.65
5811	ND1	HIS	B	98	16.798	27.505	14.135	1.00	19.24
5813	CE1	HIS	B	98	16.422	26.803	15.188	1.00	20.04
5815	NE2	HIS	B	98	15.204	26.341	14.976	1.00	19.64
5817	CD2	HIS	B	98	14.785	26.756	13.738	1.00	20.54
5819	C	HIS	B	98	14.588	29.526	10.189	1.00	18.70
5820	O	HIS	B	98	14.261	30.658	10.527	1.00	18.65
5821	N	ASP	B	99	14.949	29.218	8.946	1.00	18.55
5823	CA	ASP	B	99	14.971	30.199	7.861	1.00	18.61
5825	CB	ASP	B	99	15.515	29.530	6.605	1.00	18.44
5828	CG	ASP	B	99	15.629	30.470	5.456	1.00	18.37
5829	OD1	ASP	B	99	14.710	30.462	4.590	1.00	16.28

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5830	OD2	ASP	B	99	16.618	31.233	5.324	1.00	20.63
5831	C	ASP	B	99	13.581	30.809	7.572	1.00	18.97
5832	O	ASP	B	99	13.471	31.985	7.256	1.00	19.10
5833	N	ASP	B	100	12.537	30.007	7.703	1.00	19.32
5835	CA	ASP	B	100	11.172	30.446	7.448	1.00	20.42
5837	CB	ASP	B	100	10.283	29.224	7.206	1.00	20.29
5840	CG	ASP	B	100	10.566	28.544	5.883	1.00	20.45
5841	OD1	ASP	B	100	10.363	27.303	5.791	1.00	21.30
5842	OD2	ASP	B	100	10.981	29.158	4.885	1.00	20.64
5843	C	ASP	B	100	10.524	31.287	8.577	1.00	20.97
5844	O	ASP	B	100	9.465	31.874	8.372	1.00	21.34
5845	N	LEU	B	101	11.150	31.332	9.748	1.00	21.55
5847	CA	LEU	B	101	10.588	31.991	10.925	1.00	22.27
5849	CB	LEU	B	101	11.551	31.861	12.120	1.00	22.07
5852	CG	LEU	B	101	11.746	30.451	12.684	1.00	22.57
5854	CD1	LEU	B	101	12.901	30.397	13.690	1.00	21.96
5858	CD2	LEU	B	101	10.471	29.947	13.317	1.00	23.63
5862	C	LEU	B	101	10.313	33.470	10.646	1.00	22.59
5863	O	LEU	B	101	11.025	34.078	9.870	1.00	22.10
5864	N	PRO	B	102	9.262	34.035	11.242	1.00	23.34
5865	CA	PRO	B	102	8.959	35.467	11.096	1.00	23.88
5867	CB	PRO	B	102	7.886	35.698	12.152	1.00	23.65
5870	CG	PRO	B	102	7.151	34.422	12.154	1.00	24.22
5873	CD	PRO	B	102	8.225	33.347	12.024	1.00	23.27
5876	C	PRO	B	102	10.131	36.428	11.282	1.00	24.08
5877	O	PRO	B	102	10.211	37.387	10.523	1.00	24.64
5878	N	ALA	B	103	11.019	36.183	12.243	1.00	24.21
5880	CA	ALA	B	103	12.179	37.054	12.450	1.00	24.56
5882	CB	ALA	B	103	12.804	36.795	13.823	1.00	24.65
5886	C	ALA	B	103	13.235	36.885	11.364	1.00	24.37
5887	O	ALA	B	103	14.092	37.756	11.188	1.00	25.00
5888	N	MET	B	104	13.193	35.747	10.674	1.00	23.93
5890	CA	MET	B	104	14.111	35.445	9.578	1.00	24.35
5892	CB	MET	B	104	14.527	33.969	9.642	1.00	24.14
5895	CG	MET	B	104	15.317	33.629	10.912	1.00	26.61
5898	SD	MET	B	104	17.063	34.058	10.820	1.00	29.08
5899	CE	MET	B	104	17.584	33.058	9.452	1.00	29.15
5903	C	MET	B	104	13.463	35.845	8.237	1.00	23.69
5904	O	MET	B	104	13.310	37.040	7.995	1.00	23.79
5905	N	ASP	B	105	13.044	34.885	7.404	1.00	23.23
5907	CA	ASP	B	105	12.489	35.198	6.073	1.00	22.98
5909	CB	ASP	B	105	12.936	34.167	5.016	1.00	22.62
5912	CG	ASP	B	105	14.429	34.138	4.838	1.00	21.61
5913	OD1	ASP	B	105	14.957	33.260	4.090	1.00	18.84
5914	OD2	ASP	B	105	15.163	34.963	5.413	1.00	21.22
5915	C	ASP	B	105	10.967	35.289	6.067	1.00	23.49
5916	O	ASP	B	105	10.365	35.645	5.054	1.00	22.75
5917	N	ASP	B	106	10.348	34.950	7.185	1.00	23.98
5919	CA	ASP	B	106	8.907	35.099	7.339	1.00	25.41
5921	CB	ASP	B	106	8.567	36.597	7.503	1.00	25.60
5924	CG	ASP	B	106	7.203	36.817	8.103	1.00	27.51
5925	OD1	ASP	B	106	6.682	37.941	7.973	1.00	29.77

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5926	OD2	ASP	B	106	6.583	35.930	8.728	1.00	28.05
5927	C	ASP	B	106	8.126	34.503	6.172	1.00	25.57
5928	O	ASP	B	106	7.385	35.206	5.498	1.00	25.87
5929	N	ASP	B	107	8.309	33.203	5.936	1.00	26.04
5931	CA	ASP	B	107	7.630	32.487	4.861	1.00	25.95
5933	CB	ASP	B	107	8.641	31.685	4.032	1.00	26.04
5936	CG	ASP	B	107	9.212	32.477	2.895	1.00	26.93
5937	OD1	ASP	B	107	8.428	32.869	2.004	1.00	30.09
5938	OD2	ASP	B	107	10.426	32.755	2.786	1.00	25.96
5939	C	ASP	B	107	6.573	31.549	5.403	1.00	26.02
5940	O	ASP	B	107	6.773	30.883	6.425	1.00	26.50
5941	N	ASP	B	108	5.443	31.487	4.703	1.00	25.79
5943	CA	ASP	B	108	4.331	30.628	5.107	1.00	25.53
5945	CB	ASP	B	108	3.012	31.404	5.131	1.00	25.80
5948	CG	ASP	B	108	2.611	31.970	3.766	1.00	28.04
5949	OD1	ASP	B	108	1.460	32.426	3.651	1.00	30.10
5950	OD2	ASP	B	108	3.356	32.024	2.762	1.00	28.90
5951	C	ASP	B	108	4.183	29.359	4.260	1.00	24.50
5952	O	ASP	B	108	3.362	28.516	4.588	1.00	23.73
5953	N	LEU	B	109	4.975	29.228	3.197	1.00	23.97
5955	CA	LEU	B	109	4.939	28.054	2.323	1.00	23.69
5957	CB	LEU	B	109	4.386	28.414	0.940	1.00	24.10
5960	CG	LEU	B	109	2.907	28.201	0.569	1.00	27.09
5962	CD1	LEU	B	109	2.748	28.570	-0.917	1.00	27.23
5966	CD2	LEU	B	109	2.367	26.794	0.840	1.00	25.73
5970	C	LEU	B	109	6.329	27.462	2.103	1.00	22.98
5971	O	LEU	B	109	7.271	28.178	1.813	1.00	22.51
5972	N	ARG	B	110	6.426	26.146	2.208	1.00	22.68
5974	CA	ARG	B	110	7.609	25.422	1.776	1.00	22.37
5976	CB	ARG	B	110	8.662	25.359	2.878	1.00	22.08
5979	CG	ARG	B	110	9.916	24.624	2.441	1.00	21.74
5982	CD	ARG	B	110	11.021	24.622	3.487	1.00	19.15
5985	NE	ARG	B	110	11.586	25.949	3.737	1.00	17.98
5987	CZ	ARG	B	110	12.421	26.579	2.911	1.00	18.36
5988	NH1	ARG	B	110	12.900	27.771	3.239	1.00	19.16
5991	NH2	ARG	B	110	12.789	26.027	1.770	1.00	18.06
5994	C	ARG	B	110	7.210	24.022	1.382	1.00	22.36
5995	O	ARG	B	110	6.409	23.385	2.071	1.00	22.81
5996	N	ARG	B	111	7.789	23.549	0.283	1.00	22.18
5998	CA	ARG	B	111	7.542	22.212	-0.244	1.00	22.54
6000	CB	ARG	B	111	8.143	21.147	0.679	1.00	22.32
6003	CG	ARG	B	111	9.662	21.147	0.734	1.00	21.77
6006	CD	ARG	B	111	10.202	20.545	2.021	1.00	21.80
6009	NE	ARG	B	111	11.633	20.275	1.973	1.00	20.78
6011	CZ	ARG	B	111	12.305	19.671	2.947	1.00	20.45
6012	NH1	ARG	B	111	11.688	19.269	4.048	1.00	18.82
6015	NH2	ARG	B	111	13.608	19.464	2.826	1.00	19.98
6018	C	ARG	B	111	6.042	21.973	-0.465	1.00	23.08
6019	O	ARG	B	111	5.544	20.861	-0.338	1.00	22.39
6020	N	GLY	B	112	5.335	23.042	-0.807	1.00	23.92
6022	CA	GLY	B	112	3.921	22.975	-1.135	1.00	24.69
6025	C	GLY	B	112	3.010	23.023	0.070	1.00	24.98

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6026	O	GLY	B	112	1.808	22.978	-0.089	1.00	25.54
6027	N	LEU	B	113	3.578	23.126	1.268	1.00	25.57
6029	CA	LEU	B	113	2.813	23.045	2.508	1.00	25.94
6031	CB	LEU	B	113	3.226	21.797	3.283	1.00	26.65
6034	CG	LEU	B	113	3.068	20.468	2.548	1.00	29.36
6036	CD1	LEU	B	113	3.750	19.369	3.338	1.00	31.10
6040	CD2	LEU	B	113	1.599	20.127	2.336	1.00	31.06
6044	C	LEU	B	113	3.043	24.272	3.388	1.00	25.32
6045	O	LEU	B	113	4.027	24.999	3.216	1.00	24.34
6046	N	PRO	B	114	2.153	24.497	4.355	1.00	25.34
6047	CA	PRO	B	114	2.425	25.500	5.383	1.00	24.92
6049	CB	PRO	B	114	1.261	25.331	6.348	1.00	25.42
6052	CG	PRO	B	114	0.165	24.734	5.503	1.00	25.33
6055	CD	PRO	B	114	0.862	23.812	4.575	1.00	25.09
6058	C	PRO	B	114	3.764	25.201	6.077	1.00	24.65
6059	O	PRO	B	114	4.051	24.057	6.403	1.00	24.29
6060	N	THR	B	115	4.583	26.222	6.259	1.00	24.42
6062	CA	THR	B	115	5.850	26.062	6.966	1.00	24.49
6064	CB	THR	B	115	6.635	27.364	6.990	1.00	24.32
6066	OG1	THR	B	115	5.798	28.437	7.465	1.00	26.32
6068	CG2	THR	B	115	7.058	27.773	5.573	1.00	24.50
6072	C	THR	B	115	5.607	25.577	8.387	1.00	24.50
6073	O	THR	B	115	4.512	25.721	8.944	1.00	23.20
6074	N	CYS	B	116	6.641	24.995	8.969	1.00	24.26
6076	CA	CYS	B	116	6.537	24.419	10.297	1.00	24.93
6078	CB	CYS	B	116	7.885	23.869	10.759	1.00	24.70
6081	SG	CYS	B	116	8.346	22.384	9.881	1.00	26.74
6082	C	CYS	B	116	6.002	25.412	11.305	1.00	24.67
6083	O	CYS	B	116	5.204	25.042	12.148	1.00	25.48
6084	N	HIS	B	117	6.408	26.672	11.212	1.00	24.78
6086	CA	HIS	B	117	5.981	27.647	12.214	1.00	25.04
6088	CB	HIS	B	117	6.888	28.867	12.233	1.00	25.27
6091	CG	HIS	B	117	6.649	29.828	11.116	1.00	25.24
6092	ND1	HIS	B	117	5.983	31.018	11.293	1.00	26.70
6094	CE1	HIS	B	117	5.924	31.663	10.141	1.00	27.42
6096	NE2	HIS	B	117	6.532	30.935	9.226	1.00	26.41
6098	CD2	HIS	B	117	6.985	29.776	9.807	1.00	26.27
6100	C	HIS	B	117	4.539	28.076	12.018	1.00	25.01
6101	O	HIS	B	117	3.891	28.466	12.971	1.00	25.49
6102	N	VAL	B	118	4.051	28.021	10.784	1.00	25.12
6104	CA	VAL	B	118	2.631	28.253	10.508	1.00	25.25
6106	CB	VAL	B	118	2.394	28.567	9.018	1.00	25.46
6108	CG1	VAL	B	118	0.884	28.609	8.673	1.00	26.21
6112	CG2	VAL	B	118	3.035	29.894	8.681	1.00	25.70
6116	C	VAL	B	118	1.786	27.078	10.999	1.00	25.08
6117	O	VAL	B	118	0.821	27.285	11.720	1.00	24.86
6118	N	LYS	B	119	2.167	25.856	10.639	1.00	25.25
6120	CA	LYS	B	119	1.439	24.654	11.042	1.00	25.87
6122	CB	LYS	B	119	1.935	23.428	10.263	1.00	26.25
6125	CG	LYS	B	119	0.884	22.726	9.418	1.00	28.80
6128	CD	LYS	B	119	-0.165	22.025	10.250	1.00	31.95
6131	CE	LYS	B	119	-0.978	21.015	9.432	1.00	33.31

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6134	NZ	LYS	B	119	-1.864	21.671	8.417	1.00	34.97
6138	C	LYS	B	119	1.468	24.365	12.564	1.00	25.31
6139	O	LYS	B	119	0.445	24.061	13.161	1.00	24.99
6140	N	PHE	B	120	2.626	24.488	13.193	1.00	24.69
6142	CA	PHE	B	120	2.789	24.032	14.567	1.00	24.30
6144	CB	PHE	B	120	3.908	22.993	14.616	1.00	24.16
6147	CG	PHE	B	120	3.639	21.763	13.799	1.00	24.65
6148	CD1	PHE	B	120	2.915	20.704	14.332	1.00	26.16
6150	CE1	PHE	B	120	2.690	19.541	13.582	1.00	25.66
6152	CZ	PHE	B	120	3.192	19.441	12.311	1.00	25.37
6154	CE2	PHE	B	120	3.930	20.494	11.767	1.00	24.54
6156	CD2	PHE	B	120	4.158	21.637	12.513	1.00	25.35
6158	C	PHE	B	120	3.084	25.165	15.565	1.00	23.77
6159	O	PHE	B	120	3.155	24.927	16.752	1.00	23.66
6160	N	GLY	B	121	3.250	26.391	15.083	1.00	23.69
6162	CA	GLY	B	121	3.622	27.516	15.935	1.00	23.51
6165	C	GLY	B	121	5.130	27.773	15.955	1.00	23.55
6166	O	GLY	B	121	5.927	26.892	15.652	1.00	22.34
6167	N	GLU	B	122	5.518	28.986	16.320	1.00	23.70
6169	CA	GLU	B	122	6.934	29.381	16.314	1.00	24.67
6171	CB	GLU	B	122	7.091	30.868	16.639	1.00	24.89
6174	CG	GLU	B	122	6.990	31.777	15.427	1.00	27.84
6177	CD	GLU	B	122	7.069	33.248	15.796	1.00	30.34
6178	OE1	GLU	B	122	8.174	33.721	16.136	1.00	35.10
6179	OE2	GLU	B	122	6.033	33.931	15.743	1.00	32.39
6180	C	GLU	B	122	7.792	28.558	17.283	1.00	24.12
6181	O	GLU	B	122	8.925	28.199	16.955	1.00	23.74
6182	N	ALA	B	123	7.249	28.292	18.469	1.00	23.52
6184	CA	ALA	B	123	7.968	27.587	19.526	1.00	23.88
6186	CB	ALA	B	123	7.156	27.594	20.816	1.00	23.93
6190	C	ALA	B	123	8.287	26.159	19.098	1.00	23.98
6191	O	ALA	B	123	9.417	25.688	19.247	1.00	22.97
6192	N	ASN	B	124	7.290	25.494	18.524	1.00	23.86
6194	CA	ASN	B	124	7.484	24.159	17.980	1.00	24.09
6196	CB	ASN	B	124	6.165	23.561	17.486	1.00	24.26
6199	CG	ASN	B	124	5.365	22.896	18.601	1.00	26.12
6200	OD1	ASN	B	124	4.125	22.946	18.602	1.00	27.70
6201	ND2	ASN	B	124	6.064	22.278	19.561	1.00	23.40
6204	C	ASN	B	124	8.508	24.168	16.849	1.00	23.11
6205	O	ASN	B	124	9.294	23.250	16.750	1.00	22.29
6206	N	ALA	B	125	8.496	25.208	16.015	1.00	22.58
6208	CA	ALA	B	125	9.430	25.303	14.896	1.00	22.31
6210	CB	ALA	B	125	9.043	26.425	13.953	1.00	23.02
6214	C	ALA	B	125	10.836	25.526	15.405	1.00	21.81
6215	O	ALA	B	125	11.766	24.906	14.932	1.00	21.37
6216	N	ILE	B	126	10.985	26.419	16.371	1.00	21.15
6218	CA	ILE	B	126	12.293	26.701	16.936	1.00	20.84
6220	CB	ILE	B	126	12.177	27.795	18.007	1.00	20.71
6222	CG1	ILE	B	126	11.994	29.168	17.339	1.00	21.50
6225	CD1	ILE	B	126	11.342	30.199	18.243	1.00	22.29
6229	CG2	ILE	B	126	13.395	27.816	18.903	1.00	21.11
6233	C	ILE	B	126	12.888	25.423	17.523	1.00	19.99

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6234	O	ILE	B	126	14.037	25.072	17.234	1.00	19.91
6235	N	LEU	B	127	12.094	24.746	18.342	1.00	19.38
6237	CA	LEU	B	127	12.522	23.553	19.061	1.00	19.20
6239	CB	LEU	B	127	11.477	23.141	20.106	1.00	19.23
6242	CG	LEU	B	127	11.417	24.029	21.357	1.00	20.75
6244	CD1	LEU	B	127	12.776	24.131	22.047	1.00	22.13
6248	CD2	LEU	B	127	10.382	23.528	22.321	1.00	22.65
6252	C	LEU	B	127	12.776	22.413	18.096	1.00	19.26
6253	O	LEU	B	127	13.757	21.682	18.244	1.00	19.51
6254	N	ALA	B	128	11.926	22.286	17.082	1.00	18.61
6256	CA	ALA	B	128	12.073	21.218	16.108	1.00	19.13
6258	CB	ALA	B	128	10.873	21.183	15.181	1.00	18.64
6262	C	ALA	B	128	13.373	21.368	15.315	1.00	18.57
6263	O	ALA	B	128	14.079	20.387	15.065	1.00	18.99
6264	N	GLY	B	129	13.685	22.595	14.916	1.00	18.91
6266	CA	GLY	B	129	14.948	22.879	14.272	1.00	18.59
6269	C	GLY	B	129	16.117	22.574	15.200	1.00	18.99
6270	O	GLY	B	129	17.098	21.959	14.790	1.00	18.66
6271	N	ASP	B	130	16.001	22.986	16.459	1.00	19.11
6273	CA	ASP	B	130	17.061	22.771	17.457	1.00	19.02
6275	CB	ASP	B	130	16.652	23.327	18.829	1.00	18.48
6278	CG	ASP	B	130	16.654	24.851	18.881	1.00	20.10
6279	OD1	ASP	B	130	17.086	25.482	17.880	1.00	19.13
6280	OD2	ASP	B	130	16.221	25.488	19.889	1.00	20.44
6281	C	ASP	B	130	17.344	21.283	17.586	1.00	18.66
6282	O	ASP	B	130	18.481	20.860	17.541	1.00	18.36
6283	N	ALA	B	131	16.274	20.506	17.675	1.00	18.43
6285	CA	ALA	B	131	16.347	19.069	17.878	1.00	18.51
6287	CB	ALA	B	131	15.012	18.540	18.344	1.00	18.33
6291	C	ALA	B	131	16.808	18.315	16.629	1.00	18.44
6292	O	ALA	B	131	17.407	17.248	16.748	1.00	18.67
6293	N	LEU	B	132	16.518	18.850	15.445	1.00	18.17
6295	CA	LEU	B	132	16.970	18.235	14.207	1.00	18.20
6297	CB	LEU	B	132	16.213	18.786	12.995	1.00	18.38
6300	CG	LEU	B	132	14.853	18.138	12.732	1.00	17.74
6302	CD1	LEU	B	132	14.127	18.905	11.651	1.00	17.44
6306	CD2	LEU	B	132	15.017	16.674	12.341	1.00	18.02
6310	C	LEU	B	132	18.467	18.452	14.034	1.00	18.06
6311	O	LEU	B	132	19.167	17.572	13.544	1.00	18.16
6312	N	GLN	B	133	18.969	19.610	14.447	1.00	17.91
6314	CA	GLN	B	133	20.412	19.804	14.412	1.00	18.74
6316	CB	GLN	B	133	20.838	21.223	14.800	1.00	18.78
6319	CG	GLN	B	133	22.358	21.369	14.668	1.00	21.69
6322	CD	GLN	B	133	22.953	22.631	15.232	1.00	23.34
6323	OE1	GLN	B	133	22.274	23.644	15.458	1.00	24.32
6324	NE2	GLN	B	133	24.255	22.578	15.452	1.00	26.40
6327	C	GLN	B	133	21.094	18.762	15.319	1.00	18.33
6328	O	GLN	B	133	22.086	18.144	14.926	1.00	18.38
6329	N	THR	B	134	20.542	18.560	16.508	1.00	17.86
6331	CA	THR	B	134	21.121	17.657	17.476	1.00	18.15
6333	CB	THR	B	134	20.384	17.734	18.820	1.00	18.21
6335	OG1	THR	B	134	20.296	19.101	19.283	1.00	18.94

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6337	CG2	THR	B	134	21.169	17.017	19.864	1.00	19.06
6341	C	THR	B	134	21.060	16.225	16.950	1.00	18.22
6342	O	THR	B	134	22.014	15.474	17.106	1.00	18.09
6343	N	LEU	B	135	19.936	15.870	16.322	1.00	17.83
6345	CA	LEU	B	135	19.739	14.530	15.781	1.00	17.43
6347	CB	LEU	B	135	18.336	14.416	15.184	1.00	17.61
6350	CG	LEU	B	135	18.006	13.113	14.455	1.00	18.78
6352	CD1	LEU	B	135	18.167	11.908	15.367	1.00	18.23
6356	CD2	LEU	B	135	16.619	13.201	13.912	1.00	19.31
6360	C	LEU	B	135	20.818	14.186	14.743	1.00	16.77
6361	O	LEU	B	135	21.287	13.045	14.664	1.00	16.01
6362	N	ALA	B	136	21.243	15.179	13.970	1.00	16.82
6364	CA	ALA	B	136	22.280	14.960	12.974	1.00	16.89
6366	CB	ALA	B	136	22.581	16.241	12.231	1.00	17.47
6370	C	ALA	B	136	23.548	14.406	13.625	1.00	17.27
6371	O	ALA	B	136	24.184	13.484	13.091	1.00	17.46
6372	N	PHE	B	137	23.888	14.943	14.789	1.00	17.08
6374	CA	PHE	B	137	25.088	14.528	15.496	1.00	17.65
6376	CB	PHE	B	137	25.593	15.666	16.381	1.00	18.03
6379	CG	PHE	B	137	26.007	16.880	15.584	1.00	18.67
6380	CD1	PHE	B	137	25.230	18.019	15.566	1.00	18.86
6382	CE1	PHE	B	137	25.605	19.122	14.809	1.00	19.97
6384	CZ	PHE	B	137	26.757	19.070	14.029	1.00	19.23
6386	CE2	PHE	B	137	27.526	17.940	14.023	1.00	19.82
6388	CD2	PHE	B	137	27.140	16.835	14.788	1.00	21.06
6390	C	PHE	B	137	24.848	13.218	16.260	1.00	17.89
6391	O	PHE	B	137	25.764	12.440	16.419	1.00	17.92
6392	N	SER	B	138	23.613	12.966	16.699	1.00	18.09
6394	CA	SER	B	138	23.275	11.661	17.269	1.00	18.71
6396	CB	SER	B	138	21.839	11.634	17.769	1.00	18.28
6399	OG	SER	B	138	21.712	12.386	18.950	1.00	19.32
6401	C	SER	B	138	23.466	10.571	16.212	1.00	18.94
6402	O	SER	B	138	24.084	9.555	16.485	1.00	19.25
6403	N	ILE	B	139	22.967	10.819	15.001	1.00	19.22
6405	CA	ILE	B	139	23.123	9.884	13.890	1.00	19.25
6407	CB	ILE	B	139	22.430	10.403	12.622	1.00	19.39
6409	CG1	ILE	B	139	20.916	10.363	12.822	1.00	18.95
6412	CD1	ILE	B	139	20.144	11.100	11.805	1.00	21.43
6416	CG2	ILE	B	139	22.848	9.571	11.387	1.00	17.88
6420	C	ILE	B	139	24.606	9.609	13.612	1.00	19.87
6421	O	ILE	B	139	25.021	8.461	13.593	1.00	19.68
6422	N	LEU	B	140	25.397	10.648	13.393	1.00	19.88
6424	CA	LEU	B	140	26.799	10.451	13.025	1.00	20.40
6426	CB	LEU	B	140	27.452	11.764	12.620	1.00	20.25
6429	CG	LEU	B	140	27.071	12.298	11.246	1.00	20.51
6431	CD1	LEU	B	140	27.798	13.593	11.005	1.00	23.24
6435	CD2	LEU	B	140	27.402	11.299	10.149	1.00	21.98
6439	C	LEU	B	140	27.600	9.803	14.145	1.00	20.89
6440	O	LEU	B	140	28.572	9.088	13.876	1.00	21.00
6441	N	SER	B	141	27.211	10.045	15.396	1.00	21.26
6443	CA	SER	B	141	27.933	9.439	16.514	1.00	22.16
6445	CB	SER	B	141	27.926	10.329	17.756	1.00	21.93

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6448	OG	SER	B	141	26.615	10.552	18.225	1.00	23.99
6450	C	SER	B	141	27.456	8.023	16.856	1.00	22.90
6451	O	SER	B	141	28.248	7.250	17.390	1.00	22.85
6452	N	ASP	B	142	26.203	7.678	16.538	1.00	23.91
6454	CA	ASP	B	142	25.580	6.411	16.991	1.00	24.85
6456	CB	ASP	B	142	24.270	6.674	17.745	1.00	25.39
6459	CG	ASP	B	142	24.464	7.509	18.995	1.00	26.64
6460	OD1	ASP	B	142	23.535	8.249	19.365	1.00	25.98
6461	OD2	ASP	B	142	25.516	7.497	19.667	1.00	29.60
6462	C	ASP	B	142	25.262	5.407	15.890	1.00	25.42
6463	O	ASP	B	142	25.185	4.202	16.158	1.00	25.21
6464	N	ALA	B	143	25.052	5.887	14.663	1.00	25.69
6466	CA	ALA	B	143	24.533	5.031	13.592	1.00	26.20
6468	CB	ALA	B	143	24.187	5.840	12.367	1.00	26.13
6472	C	ALA	B	143	25.542	3.965	13.226	1.00	26.52
6473	O	ALA	B	143	26.739	4.190	13.292	1.00	26.08
6474	N	ASP	B	144	25.051	2.790	12.862	1.00	27.00
6476	CA	ASP	B	144	25.908	1.760	12.308	1.00	27.79
6478	CB	ASP	B	144	25.084	0.487	12.088	1.00	28.61
6481	CG	ASP	B	144	25.935	-0.733	11.853	1.00	30.23
6482	OD1	ASP	B	144	27.147	-0.714	12.160	1.00	33.26
6483	OD2	ASP	B	144	25.452	-1.776	11.358	1.00	34.68
6484	C	ASP	B	144	26.531	2.247	10.992	1.00	27.76
6485	O	ASP	B	144	25.825	2.652	10.050	1.00	27.93
6486	N	MET	B	145	27.856	2.247	10.951	1.00	27.25
6488	CA	MET	B	145	28.612	2.526	9.743	1.00	27.33
6490	CB	MET	B	145	29.181	3.936	9.772	1.00	26.88
6493	CG	MET	B	145	28.129	5.014	9.664	1.00	26.79
6496	SD	MET	B	145	28.859	6.646	9.270	1.00	27.26
6497	CE	MET	B	145	29.830	6.916	10.701	1.00	23.05
6501	C	MET	B	145	29.737	1.508	9.657	1.00	27.62
6502	O	MET	B	145	30.895	1.812	9.936	1.00	26.26
6503	N	PRO	B	146	29.393	0.291	9.256	1.00	28.79
6504	CA	PRO	B	146	30.354	-0.815	9.234	1.00	29.73
6506	CB	PRO	B	146	29.669	-1.832	8.320	1.00	29.99
6509	CG	PRO	B	146	28.228	-1.630	8.593	1.00	29.30
6512	CD	PRO	B	146	28.060	-0.137	8.799	1.00	29.11
6515	C	PRO	B	146	31.733	-0.464	8.696	1.00	30.46
6516	O	PRO	B	146	32.732	-0.822	9.317	1.00	30.83
6517	N	GLU	B	147	31.801	0.253	7.586	1.00	31.81
6519	CA	GLU	B	147	33.089	0.431	6.905	1.00	33.36
6521	CB	GLU	B	147	32.889	0.840	5.426	1.00	34.57
6524	CG	GLU	B	147	31.629	0.304	4.730	1.00	37.40
6527	CD	GLU	B	147	31.768	0.264	3.209	1.00	41.76
6528	OE1	GLU	B	147	30.918	-0.387	2.543	1.00	42.19
6529	OE2	GLU	B	147	32.733	0.877	2.676	1.00	43.49
6530	C	GLU	B	147	34.030	1.449	7.587	1.00	32.65
6531	O	GLU	B	147	35.172	1.605	7.155	1.00	33.17
6532	N	VAL	B	148	33.572	2.099	8.660	1.00	31.25
6534	CA	VAL	B	148	34.097	3.410	9.043	1.00	30.18
6536	CB	VAL	B	148	32.970	4.456	9.012	1.00	30.21
6538	CG1	VAL	B	148	33.501	5.842	9.381	1.00	29.95

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6542	CG2	VAL	B	148	32.310	4.467	7.634	1.00	30.63
6546	C	VAL	B	148	34.767	3.425	10.417	1.00	28.89
6547	O	VAL	B	148	34.131	3.174	11.431	1.00	27.43
6548	N	SER	B	149	36.057	3.755	10.435	1.00	28.02
6550	CA	SER	B	149	36.806	3.836	11.681	1.00	27.32
6552	CB	SER	B	149	38.302	4.022	11.413	1.00	27.23
6555	OG	SER	B	149	38.554	5.276	10.811	1.00	25.67
6557	C	SER	B	149	36.295	4.984	12.540	1.00	27.03
6558	O	SER	B	149	35.651	5.906	12.045	1.00	26.50
6559	N	ASP	B	150	36.601	4.899	13.831	1.00	26.71
6561	CA	ASP	B	150	36.236	5.914	14.810	1.00	26.65
6563	CB	ASP	B	150	36.729	5.509	16.194	1.00	26.35
6566	CG	ASP	B	150	35.776	4.575	16.906	1.00	28.03
6567	OD1	ASP	B	150	36.086	4.216	18.054	1.00	30.17
6568	OD2	ASP	B	150	34.692	4.157	16.424	1.00	29.62
6569	C	ASP	B	150	36.824	7.253	14.407	1.00	26.23
6570	O	ASP	B	150	36.146	8.269	14.454	1.00	25.29
6571	N	ARG	B	151	38.077	7.229	13.970	1.00	26.28
6573	CA	ARG	B	151	38.745	8.409	13.442	1.00	26.55
6575	CB	ARG	B	151	40.172	8.069	13.019	1.00	27.45
6578	CG	ARG	B	151	41.099	9.254	13.054	1.00	30.78
6581	CD	ARG	B	151	41.726	9.500	14.416	1.00	34.73
6584	NE	ARG	B	151	41.001	10.520	15.179	1.00	38.97
6586	CZ	ARG	B	151	41.152	11.835	15.043	1.00	42.64
6587	NH1	ARG	B	151	42.000	12.354	14.148	1.00	45.06
6590	NH2	ARG	B	151	40.435	12.651	15.801	1.00	43.15
6593	C	ARG	B	151	38.004	9.052	12.268	1.00	25.50
6594	O	ARG	B	151	37.870	10.265	12.211	1.00	25.19
6595	N	ASP	B	152	37.540	8.252	11.315	1.00	24.83
6597	CA	ASP	B	152	36.823	8.813	10.171	1.00	24.18
6599	CB	ASP	B	152	36.747	7.809	9.030	1.00	24.78
6602	CG	ASP	B	152	38.117	7.499	8.443	1.00	26.32
6603	OD1	ASP	B	152	39.074	8.280	8.679	1.00	29.38
6604	OD2	ASP	B	152	38.329	6.479	7.758	1.00	28.43
6605	C	ASP	B	152	35.427	9.290	10.562	1.00	22.75
6606	O	ASP	B	152	34.923	10.240	10.007	1.00	22.39
6607	N	ARG	B	153	34.810	8.619	11.521	1.00	21.86
6609	CA	ARG	B	153	33.532	9.053	12.064	1.00	20.79
6611	CB	ARG	B	153	33.022	8.054	13.088	1.00	20.74
6614	CG	ARG	B	153	31.647	8.375	13.651	1.00	20.82
6617	CD	ARG	B	153	31.205	7.399	14.704	1.00	20.94
6620	NE	ARG	B	153	30.980	6.045	14.173	1.00	22.48
6622	CZ	ARG	B	153	29.790	5.511	13.895	1.00	23.71
6623	NH1	ARG	B	153	29.723	4.256	13.448	1.00	25.23
6626	NH2	ARG	B	153	28.671	6.205	14.046	1.00	20.67
6629	C	ARG	B	153	33.676	10.426	12.714	1.00	20.58
6630	O	ARG	B	153	32.833	11.297	12.519	1.00	18.98
6631	N	ILE	B	154	34.752	10.610	13.483	1.00	20.29
6633	CA	ILE	B	154	35.016	11.891	14.124	1.00	20.38
6635	CB	ILE	B	154	36.209	11.808	15.090	1.00	20.21
6637	CG1	ILE	B	154	35.848	10.962	16.319	1.00	20.02
6640	CD1	ILE	B	154	37.077	10.390	17.035	1.00	21.78

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6644	CG2	ILE	B	154	36.656	13.203	15.514	1.00	21.46
6648	C	ILE	B	154	35.247	12.940	13.051	1.00	20.53
6649	O	ILE	B	154	34.737	14.018	13.158	1.00	20.41
6650	N	SER	B	155	35.976	12.593	11.996	1.00	21.07
6652	CA	SER	B	155	36.182	13.485	10.864	1.00	21.78
6654	CB	SER	B	155	37.097	12.822	9.824	1.00	22.36
6657	OG	SER	B	155	38.452	13.117	10.107	1.00	25.91
6659	C	SER	B	155	34.867	13.924	10.186	1.00	21.46
6660	O	SER	B	155	34.771	15.053	9.711	1.00	21.56
6661	N	MET	B	156	33.886	13.029	10.125	1.00	21.47
6663	CA	MET	B	156	32.569	13.337	9.576	1.00	21.23
6665	CB	MET	B	156	31.726	12.079	9.403	1.00	21.94
6668	CG	MET	B	156	32.183	11.183	8.281	1.00	24.79
6671	SD	MET	B	156	31.189	9.677	8.224	1.00	31.73
6672	CE	MET	B	156	32.337	8.674	7.553	1.00	32.04
6676	C	MET	B	156	31.815	14.278	10.480	1.00	20.18
6677	O	MET	B	156	31.164	15.191	10.005	1.00	20.12
6678	N	ILE	B	157	31.894	14.045	11.782	1.00	20.00
6680	CA	ILE	B	157	31.238	14.915	12.744	1.00	19.69
6682	CB	ILE	B	157	31.290	14.326	14.178	1.00	19.62
6684	CG1	ILE	B	157	30.466	13.047	14.259	1.00	19.47
6687	CD1	ILE	B	157	30.741	12.182	15.483	1.00	21.29
6691	CG2	ILE	B	157	30.763	15.332	15.177	1.00	18.69
6695	C	ILE	B	157	31.878	16.289	12.688	1.00	19.80
6696	O	ILE	B	157	31.182	17.300	12.684	1.00	20.00
6697	N	SER	B	158	33.204	16.340	12.640	1.00	19.73
6699	CA	SER	B	158	33.894	17.619	12.559	1.00	19.44
6701	CB	SER	B	158	35.410	17.419	12.507	1.00	19.53
6704	OG	SER	B	158	36.053	18.665	12.347	1.00	19.74
6706	C	SER	B	158	33.469	18.403	11.325	1.00	19.46
6707	O	SER	B	158	33.193	19.587	11.408	1.00	18.61
6708	N	GLU	B	159	33.429	17.734	10.181	1.00	20.02
6710	CA	GLU	B	159	33.084	18.384	8.932	1.00	20.06
6712	CB	GLU	B	159	33.224	17.423	7.757	1.00	20.49
6715	CG	GLU	B	159	32.576	17.922	6.472	1.00	21.89
6718	CD	GLU	B	159	33.103	19.290	6.041	1.00	23.61
6719	OE1	GLU	B	159	34.281	19.584	6.322	1.00	24.99
6720	OE2	GLU	B	159	32.347	20.067	5.426	1.00	25.28
6721	C	GLU	B	159	31.658	18.934	8.990	1.00	19.72
6722	O	GLU	B	159	31.422	20.062	8.577	1.00	19.69
6723	N	LEU	B	160	30.720	18.140	9.494	1.00	18.90
6725	CA	LEU	B	160	29.324	18.550	9.526	1.00	18.94
6727	CB	LEU	B	160	28.406	17.404	9.956	1.00	18.87
6730	CG	LEU	B	160	26.915	17.695	9.771	1.00	19.53
6732	CD1	LEU	B	160	26.644	18.166	8.357	1.00	19.83
6736	CD2	LEU	B	160	26.076	16.470	10.093	1.00	20.63
6740	C	LEU	B	160	29.158	19.736	10.458	1.00	18.48
6741	O	LEU	B	160	28.486	20.694	10.130	1.00	18.99
6742	N	ALA	B	161	29.803	19.673	11.612	1.00	18.69
6744	CA	ALA	B	161	29.769	20.773	12.560	1.00	18.51
6746	CB	ALA	B	161	30.446	20.384	13.872	1.00	18.21
6750	C	ALA	B	161	30.377	22.045	11.970	1.00	19.04

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6751	O	ALA	B	161	29.749	23.095	12.012	1.00	18.97
6752	N	SER	B	162	31.573	21.976	11.387	1.00	19.49
6754	CA	SER	B	162	32.161	23.190	10.838	1.00	19.97
6756	CB	SER	B	162	33.630	22.988	10.472	1.00	20.60
6759	OG	SER	B	162	33.756	21.975	9.518	1.00	24.18
6761	C	SER	B	162	31.348	23.734	9.643	1.00	19.40
6762	O	SER	B	162	31.186	24.958	9.482	1.00	18.70
6763	N	ALA	B	163	30.813	22.832	8.825	1.00	19.19
6765	CA	ALA	B	163	29.974	23.225	7.690	1.00	18.98
6767	CB	ALA	B	163	29.671	22.011	6.798	1.00	19.19
6771	C	ALA	B	163	28.672	23.907	8.081	1.00	18.85
6772	O	ALA	B	163	28.157	24.742	7.341	1.00	19.30
6773	N	SER	B	164	28.135	23.537	9.228	1.00	18.81
6775	CA	SER	B	164	26.788	23.931	9.638	1.00	18.52
6777	CB	SER	B	164	26.128	22.787	10.405	1.00	18.45
6780	OG	SER	B	164	26.073	21.610	9.622	1.00	18.06
6782	C	SER	B	164	26.780	25.159	10.526	1.00	18.48
6783	O	SER	B	164	25.779	25.828	10.630	1.00	18.20
6784	N	GLY	B	165	27.902	25.438	11.177	1.00	19.42
6786	CA	GLY	B	165	27.950	26.481	12.175	1.00	19.70
6789	C	GLY	B	165	28.359	27.810	11.598	1.00	20.33
6790	O	GLY	B	165	28.096	28.122	10.441	1.00	19.41
6791	N	ILE	B	166	29.018	28.604	12.424	1.00	21.45
6793	CA	ILE	B	166	29.348	29.976	12.074	1.00	22.91
6795	CB	ILE	B	166	29.846	30.707	13.354	1.00	23.50
6797	CG1	ILE	B	166	29.737	32.206	13.173	1.00	25.77
6800	CD1	ILE	B	166	28.314	32.688	13.353	1.00	25.49
6804	CG2	ILE	B	166	31.229	30.245	13.727	1.00	24.89
6808	C	ILE	B	166	30.354	30.068	10.916	1.00	22.56
6809	O	ILE	B	166	30.335	31.016	10.141	1.00	22.77
6810	N	ALA	B	167	31.207	29.059	10.771	1.00	22.49
6812	CA	ALA	B	167	32.152	29.006	9.656	1.00	22.06
6814	CB	ALA	B	167	33.324	28.148	10.023	1.00	21.92
6818	C	ALA	B	167	31.490	28.488	8.383	1.00	22.04
6819	O	ALA	B	167	32.146	28.318	7.376	1.00	22.97
6820	N	GLY	B	168	30.181	28.252	8.430	1.00	21.24
6822	CA	GLY	B	168	29.464	27.684	7.313	1.00	20.53
6825	C	GLY	B	168	28.034	28.189	7.292	1.00	20.28
6826	O	GLY	B	168	27.804	29.394	7.295	1.00	19.03
6827	N	MET	B	169	27.082	27.265	7.340	1.00	20.39
6829	CA	MET	B	169	25.676	27.559	7.077	1.00	21.14
6831	CB	MET	B	169	24.855	26.298	7.278	1.00	21.40
6834	CG	MET	B	169	23.410	26.392	6.837	1.00	23.14
6837	SD	MET	B	169	22.401	27.153	8.090	1.00	26.74
6838	CE	MET	B	169	22.407	25.862	9.410	1.00	26.17
6842	C	MET	B	169	25.147	28.696	7.938	1.00	21.67
6843	O	MET	B	169	24.556	29.644	7.436	1.00	21.21
6844	N	CYS	B	170	25.367	28.594	9.239	1.00	22.13
6846	CA	CYS	B	170	24.827	29.556	10.170	1.00	22.50
6848	CB	BCYS	B	170	25.042	29.096	11.614	0.35	22.49
6849	CB	ACYS	B	170	25.010	29.057	11.596	0.65	22.96
6854	SG	BCYS	B	170	23.609	28.307	12.340	0.35	22.05

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6855	SG	ACYS	B	170	24.028	29.996	12.749	0.65	25.42
6856	C	CYS	B	170	25.460	30.935	9.997	1.00	21.94
6857	O	CYS	B	170	24.775	31.934	10.105	1.00	22.08
6858	N	GLY	B	171	26.767	30.980	9.758	1.00	21.27
6860	CA	GLY	B	171	27.453	32.231	9.504	1.00	21.35
6863	C	GLY	B	171	26.951	32.858	8.218	1.00	20.97
6864	O	GLY	B	171	26.839	34.081	8.111	1.00	20.81
6865	N	GLY	B	172	26.643	32.009	7.249	1.00	20.08
6867	CA	GLY	B	172	26.027	32.440	6.009	1.00	19.62
6870	C	GLY	B	172	24.641	33.007	6.215	1.00	19.25
6871	O	GLY	B	172	24.288	34.011	5.605	1.00	18.27
6872	N	GLN	B	173	23.858	32.380	7.084	1.00	18.75
6874	CA	GLN	B	173	22.535	32.890	7.404	1.00	19.22
6876	CB	GLN	B	173	21.787	31.947	8.348	1.00	19.67
6879	CG	GLN	B	173	21.349	30.652	7.682	1.00	20.18
6882	CD	GLN	B	173	20.333	30.899	6.597	1.00	20.92
6883	OE1	GLN	B	173	20.701	31.297	5.496	1.00	21.77
6884	NE2	GLN	B	173	19.047	30.712	6.914	1.00	19.90
6887	C	GLN	B	173	22.632	34.281	8.002	1.00	19.31
6888	O	GLN	B	173	21.805	35.146	7.691	1.00	18.98
6889	N	ALA	B	174	23.667	34.503	8.810	1.00	19.26
6891	CA	ALA	B	174	23.894	35.813	9.437	1.00	20.09
6893	CB	ALA	B	174	24.956	35.725	10.526	1.00	19.57
6897	C	ALA	B	174	24.292	36.845	8.387	1.00	20.47
6898	O	ALA	B	174	23.826	37.969	8.440	1.00	21.60
6899	N	LEU	B	175	25.143	36.464	7.436	1.00	21.00
6901	CA	LEU	B	175	25.561	37.384	6.371	1.00	21.21
6903	CB	LEU	B	175	26.646	36.753	5.497	1.00	21.41
6906	CG	LEU	B	175	28.026	36.557	6.121	1.00	23.45
6908	CD1	LEU	B	175	28.948	35.855	5.138	1.00	24.47
6912	CD2	LEU	B	175	28.630	37.913	6.562	1.00	24.78
6916	C	LEU	B	175	24.358	37.776	5.519	1.00	21.36
6917	O	LEU	B	175	24.210	38.942	5.118	1.00	20.88
6918	N	ASP	B	176	23.498	36.794	5.258	1.00	21.82
6920	CA	ASP	B	176	22.291	36.980	4.466	1.00	22.30
6922	CB	ASP	B	176	21.615	35.625	4.252	1.00	22.47
6925	CG	ASP	B	176	20.205	35.739	3.779	1.00	21.57
6926	OD1	ASP	B	176	19.938	35.449	2.588	1.00	22.94
6927	OD2	ASP	B	176	19.281	36.072	4.540	1.00	25.04
6928	C	ASP	B	176	21.356	37.989	5.138	1.00	23.38
6929	O	ASP	B	176	20.856	38.927	4.499	1.00	23.61
6930	N	LEU	B	177	21.131	37.814	6.429	1.00	24.61
6932	CA	LEU	B	177	20.296	38.751	7.181	1.00	26.08
6934	CB	LEU	B	177	20.112	38.267	8.621	1.00	26.86
6937	CG	LEU	B	177	18.842	37.475	8.968	1.00	28.65
6939	CD1	LEU	B	177	18.029	36.990	7.768	1.00	30.94
6943	CD2	LEU	B	177	19.243	36.330	9.825	1.00	29.29
6947	C	LEU	B	177	20.891	40.147	7.193	1.00	26.38
6948	O	LEU	B	177	20.176	41.134	7.048	1.00	27.18
6949	N	ASP	B	178	22.203	40.228	7.355	1.00	27.07
6951	CA	ASP	B	178	22.893	41.513	7.389	1.00	27.97
6953	CB	ASP	B	178	24.336	41.337	7.864	1.00	28.49

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6956	CG	ASP	B	178	24.926	42.624	8.427	1.00	31.55
6957	OD1	ASP	B	178	25.937	43.106	7.874	1.00	34.43
6958	OD2	ASP	B	178	24.447	43.218	9.419	1.00	36.43
6959	C	ASP	B	178	22.865	42.228	6.034	1.00	27.98
6960	O	ASP	B	178	22.853	43.454	5.993	1.00	27.47
6961	N	ALA	B	179	22.828	41.462	4.936	1.00	27.64
6963	CA	ALA	B	179	22.818	42.026	3.576	1.00	27.64
6965	CB	ALA	B	179	23.397	41.024	2.579	1.00	27.26
6969	C	ALA	B	179	21.415	42.474	3.118	1.00	27.90
6970	O	ALA	B	179	21.288	43.142	2.109	1.00	27.38
6971	N	GLU	B	180	20.374	42.097	3.852	1.00	28.50
6973	CA	GLU	B	180	19.006	42.515	3.535	1.00	29.13
6975	CB	GLU	B	180	18.031	42.069	4.629	1.00	29.71
6978	CG	GLU	B	180	17.071	40.969	4.234	1.00	31.66
6981	CD	GLU	B	180	16.175	40.534	5.384	1.00	33.14
6982	OE1	GLU	B	180	15.509	41.400	5.995	1.00	35.30
6983	OE2	GLU	B	180	16.149	39.324	5.684	1.00	32.62
6984	C	GLU	B	180	18.922	44.041	3.418	1.00	29.49
6985	O	GLU	B	180	19.290	44.755	4.348	1.00	28.60
6986	N	GLY	B	181	18.454	44.518	2.264	1.00	29.61
6988	CA	GLY	B	181	18.279	45.935	1.997	1.00	29.83
6991	C	GLY	B	181	19.560	46.670	1.658	1.00	30.04
6992	O	GLY	B	181	19.532	47.871	1.420	1.00	30.48
6993	N	LYS	B	182	20.681	45.954	1.622	1.00	30.21
6995	CA	LYS	B	182	21.992	46.573	1.506	1.00	30.46
6997	CB	LYS	B	182	22.959	45.982	2.526	1.00	30.97
7000	CG	LYS	B	182	22.593	46.287	3.973	1.00	32.58
7003	CD	LYS	B	182	23.830	46.343	4.864	1.00	34.32
7006	CE	LYS	B	182	23.490	46.882	6.259	1.00	35.98
7009	NZ	LYS	B	182	23.339	45.804	7.290	1.00	36.88
7013	C	LYS	B	182	22.573	46.427	0.116	1.00	30.22
7014	O	LYS	B	182	23.559	47.083	-0.203	1.00	30.23
7015	N	HIS	B	183	21.984	45.555	-0.700	1.00	29.28
7017	CA	HIS	B	183	22.375	45.441	-2.093	1.00	29.34
7019	CB	HIS	B	183	21.892	46.684	-2.856	1.00	29.70
7022	CG	HIS	B	183	20.410	46.833	-2.832	1.00	30.08
7023	ND1	HIS	B	183	19.699	47.003	-1.668	1.00	32.28
7025	CE1	HIS	B	183	18.412	47.068	-1.942	1.00	31.16
7027	NE2	HIS	B	183	18.261	46.940	-3.244	1.00	32.50
7029	CD2	HIS	B	183	19.497	46.782	-3.821	1.00	32.70
7031	C	HIS	B	183	23.887	45.297	-2.191	1.00	28.93
7032	O	HIS	B	183	24.558	46.097	-2.847	1.00	29.19
7033	N	VAL	B	184	24.415	44.274	-1.522	1.00	27.85
7035	CA	VAL	B	184	25.850	44.103	-1.417	1.00	27.29
7037	CB	VAL	B	184	26.247	43.065	-0.319	1.00	27.33
7039	CG1	VAL	B	184	25.636	43.452	1.052	1.00	27.10
7043	CG2	VAL	B	184	25.860	41.634	-0.722	1.00	27.05
7047	C	VAL	B	184	26.419	43.723	-2.779	1.00	26.86
7048	O	VAL	B	184	25.733	43.075	-3.577	1.00	26.12
7049	N	PRO	B	185	27.663	44.126	-3.051	1.00	26.31
7050	CA	PRO	B	185	28.314	43.792	-4.319	1.00	26.16
7052	CB	PRO	B	185	29.596	44.623	-4.284	1.00	26.24

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7055	CG	PRO	B	185	29.892	44.801	-2.835	1.00	26.65
7058	CD	PRO	B	185	28.552	44.905	-2.168	1.00	26.81
7061	C	PRO	B	185	28.646	42.297	-4.436	1.00	25.85
7062	O	PRO	B	185	28.521	41.553	-3.475	1.00	24.67
7063	N	LEU	B	186	29.106	41.908	-5.616	1.00	26.22
7065	CA	LEU	B	186	29.284	40.509	-6.002	1.00	26.42
7067	CB	LEU	B	186	29.859	40.422	-7.424	1.00	26.65
7070	CG	LEU	B	186	29.462	39.279	-8.371	1.00	28.07
7072	CD1	LEU	B	186	30.565	39.033	-9.399	1.00	29.61
7076	CD2	LEU	B	186	29.105	38.004	-7.671	1.00	28.33
7080	C	LEU	B	186	30.183	39.726	-5.048	1.00	26.27
7081	O	LEU	B	186	29.890	38.580	-4.737	1.00	25.80
7082	N	ASP	B	187	31.286	40.317	-4.590	1.00	26.90
7084	CA	ASP	B	187	32.198	39.558	-3.721	1.00	27.11
7086	CB	ASP	B	187	33.567	40.236	-3.526	1.00	27.85
7089	CG	ASP	B	187	33.480	41.648	-2.951	1.00	30.82
7090	OD1	ASP	B	187	34.555	42.173	-2.574	1.00	36.51
7091	OD2	ASP	B	187	32.435	42.331	-2.848	1.00	35.53
7092	C	ASP	B	187	31.554	39.180	-2.380	1.00	26.24
7093	O	ASP	B	187	31.729	38.053	-1.900	1.00	25.65
7094	N	ALA	B	188	30.809	40.117	-1.799	1.00	25.42
7096	CA	ALA	B	188	30.097	39.892	-0.548	1.00	24.85
7098	CB	ALA	B	188	29.610	41.221	0.019	1.00	24.84
7102	C	ALA	B	188	28.915	38.951	-0.774	1.00	24.38
7103	O	ALA	B	188	28.578	38.154	0.081	1.00	24.14
7104	N	LEU	B	189	28.291	39.059	-1.942	1.00	24.33
7106	CA	LEU	B	189	27.156	38.230	-2.286	1.00	24.42
7108	CB	LEU	B	189	26.530	38.741	-3.577	1.00	24.99
7111	CG	LEU	B	189	25.509	37.865	-4.268	1.00	25.94
7113	CD1	LEU	B	189	24.317	37.593	-3.350	1.00	26.65
7117	CD2	LEU	B	189	25.072	38.566	-5.566	1.00	26.30
7121	C	LEU	B	189	27.607	36.783	-2.435	1.00	23.85
7122	O	LEU	B	189	26.965	35.863	-1.918	1.00	23.56
7123	N	GLU	B	190	28.727	36.590	-3.115	1.00	23.22
7125	CA	GLU	B	190	29.301	35.269	-3.280	1.00	23.29
7127	CB	GLU	B	190	30.566	35.331	-4.135	1.00	23.75
7130	CG	GLU	B	190	31.070	33.963	-4.535	1.00	25.63
7133	CD	GLU	B	190	32.356	33.994	-5.339	1.00	28.46
7134	OE1	GLU	B	190	33.201	33.121	-5.090	1.00	31.64
7135	OE2	GLU	B	190	32.522	34.854	-6.226	1.00	32.12
7136	C	GLU	B	190	29.625	34.655	-1.917	1.00	22.85
7137	O	GLU	B	190	29.434	33.459	-1.699	1.00	20.62
7138	N	ARG	B	191	30.114	35.490	-1.009	1.00	22.57
7140	CA	ARG	B	191	30.499	35.041	0.315	1.00	22.97
7142	CB	ARG	B	191	31.169	36.171	1.077	1.00	23.59
7145	CG	ARG	B	191	31.646	35.789	2.444	1.00	26.56
7148	CD	ARG	B	191	32.707	36.714	3.004	1.00	31.42
7151	NE	ARG	B	191	32.158	37.666	3.962	1.00	35.82
7153	CZ	ARG	B	191	32.874	38.304	4.891	1.00	38.83
7154	NH1	ARG	B	191	34.184	38.105	5.012	1.00	39.90
7157	NH2	ARG	B	191	32.270	39.150	5.712	1.00	40.92
7160	C	ARG	B	191	29.282	34.546	1.087	1.00	21.94

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7161	O	ARG	B	191	29.357	33.536	1.770	1.00	22.24
7162	N	ILE	B	192	28.160	35.246	0.947	1.00	21.11
7164	CA	ILE	B	192	26.916	34.836	1.574	1.00	19.99
7166	CB	ILE	B	192	25.763	35.775	1.186	1.00	19.92
7168	CG1	ILE	B	192	25.925	37.151	1.835	1.00	20.88
7171	CD1	ILE	B	192	25.092	38.196	1.195	1.00	21.97
7175	CG2	ILE	B	192	24.408	35.196	1.598	1.00	19.49
7179	C	ILE	B	192	26.589	33.421	1.107	1.00	19.95
7180	O	ILE	B	192	26.387	32.538	1.914	1.00	19.48
7181	N	HIS	B	193	26.542	33.231	-0.207	1.00	19.56
7183	CA	HIS	B	193	26.027	31.999	-0.802	1.00	18.94
7185	CB	HIS	B	193	25.801	32.209	-2.298	1.00	19.11
7188	CG	HIS	B	193	24.584	33.024	-2.606	1.00	17.67
7189	ND1	HIS	B	193	23.920	33.755	-1.647	1.00	19.83
7191	CE1	HIS	B	193	22.873	34.349	-2.191	1.00	19.06
7193	NE2	HIS	B	193	22.821	34.013	-3.467	1.00	19.16
7195	CD2	HIS	B	193	23.882	33.186	-3.754	1.00	19.39
7197	C	HIS	B	193	26.913	30.802	-0.543	1.00	18.45
7198	O	HIS	B	193	26.422	29.700	-0.294	1.00	18.16
7199	N	ARG	B	194	28.221	31.017	-0.579	1.00	18.21
7201	CA	ARG	B	194	29.157	29.954	-0.301	1.00	18.14
7203	CB	ARG	B	194	30.582	30.396	-0.588	1.00	18.28
7206	CG	ARG	B	194	30.894	30.549	-2.059	1.00	18.14
7209	CD	ARG	B	194	32.368	30.534	-2.332	1.00	19.86
7212	NE	ARG	B	194	32.685	30.696	-3.740	1.00	20.51
7214	CZ	ARG	B	194	32.656	29.723	-4.648	1.00	23.08
7215	NH1	ARG	B	194	32.326	28.482	-4.320	1.00	24.68
7218	NH2	ARG	B	194	32.981	29.995	-5.900	1.00	25.18
7221	C	ARG	B	194	29.003	29.465	1.143	1.00	18.28
7222	O	ARG	B	194	29.037	28.267	1.392	1.00	18.15
7223	N	HIS	B	195	28.782	30.390	2.079	1.00	18.49
7225	CA	HIS	B	195	28.558	30.036	3.479	1.00	18.76
7227	CB	HIS	B	195	28.786	31.251	4.390	1.00	18.80
7230	CG	HIS	B	195	30.224	31.612	4.533	1.00	19.89
7231	ND1	HIS	B	195	30.934	32.241	3.533	1.00	21.51
7233	CE1	HIS	B	195	32.186	32.408	3.925	1.00	21.57
7235	NE2	HIS	B	195	32.311	31.910	5.142	1.00	21.37
7237	CD2	HIS	B	195	31.103	31.395	5.541	1.00	21.40
7239	C	HIS	B	195	27.170	29.430	3.697	1.00	18.88
7240	O	HIS	B	195	27.050	28.298	4.182	1.00	19.41
7241	N	LYS	B	196	26.117	30.122	3.293	1.00	18.32
7243	CA	LYS	B	196	24.778	29.672	3.686	1.00	18.29
7245	CB	LYS	B	196	23.725	30.764	3.506	1.00	18.11
7248	CG	LYS	B	196	23.241	31.027	2.080	1.00	17.45
7251	CD	LYS	B	196	22.081	32.049	2.131	1.00	17.15
7254	CE	LYS	B	196	21.634	32.547	0.768	1.00	15.61
7257	NZ	LYS	B	196	20.235	33.122	0.794	1.00	15.01
7261	C	LYS	B	196	24.322	28.389	3.006	1.00	18.44
7262	O	LYS	B	196	23.466	27.688	3.541	1.00	18.43
7263	N	THR	B	197	24.898	28.098	1.841	1.00	17.92
7265	CA	THR	B	197	24.454	27.009	0.983	1.00	18.22
7267	CB	THR	B	197	23.686	27.598	-0.203	1.00	17.81

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7269	OG1	THR	B	197	22.429	28.070	0.261	1.00	18.26
7271	CG2	THR	B	197	23.322	26.539	-1.246	1.00	18.58
7275	C	THR	B	197	25.601	26.129	0.504	1.00	17.84
7276	O	THR	B	197	25.482	24.907	0.475	1.00	18.55
7277	N	GLY	B	198	26.703	26.746	0.104	1.00	17.60
7279	CA	GLY	B	198	27.854	26.006	-0.358	1.00	17.04
7282	C	GLY	B	198	28.469	25.112	0.708	1.00	16.72
7283	O	GLY	B	198	28.863	23.993	0.415	1.00	15.65
7284	N	ALA	B	199	28.523	25.581	1.951	1.00	16.19
7286	CA	ALA	B	199	29.239	24.837	2.993	1.00	16.23
7288	CB	ALA	B	199	29.265	25.611	4.271	1.00	16.00
7292	C	ALA	B	199	28.633	23.441	3.200	1.00	16.09
7293	O	ALA	B	199	29.357	22.445	3.312	1.00	16.00
7294	N	LEU	B	200	27.309	23.363	3.200	1.00	15.80
7296	CA	LEU	B	200	26.623	22.126	3.536	1.00	16.20
7298	CB	LEU	B	200	25.202	22.408	4.018	1.00	16.05
7301	CG	LEU	B	200	24.363	21.238	4.540	1.00	18.16
7303	CD1	LEU	B	200	25.019	20.573	5.727	1.00	18.85
7307	CD2	LEU	B	200	22.989	21.735	4.928	1.00	18.03
7311	C	LEU	B	200	26.593	21.206	2.332	1.00	16.19
7312	O	LEU	B	200	26.544	19.993	2.479	1.00	15.79
7313	N	ILE	B	201	26.615	21.769	1.136	1.00	16.74
7315	CA	ILE	B	201	26.723	20.928	-0.052	1.00	17.10
7317	CB	ILE	B	201	26.341	21.713	-1.305	1.00	17.41
7319	CG1	ILE	B	201	24.806	21.764	-1.403	1.00	18.09
7322	CD1	ILE	B	201	24.283	22.985	-2.120	1.00	19.65
7326	CG2	ILE	B	201	26.936	21.073	-2.581	1.00	16.41
7330	C	ILE	B	201	28.130	20.312	-0.110	1.00	17.27
7331	O	ILE	B	201	28.289	19.126	-0.436	1.00	16.47
7332	N	ARG	B	202	29.139	21.098	0.240	1.00	17.03
7334	CA	ARG	B	202	30.468	20.539	0.389	1.00	17.33
7336	CB	ARG	B	202	31.516	21.598	0.645	1.00	17.65
7339	CG	ARG	B	202	32.956	20.997	0.625	1.00	18.08
7342	CD	ARG	B	202	34.038	22.029	0.637	1.00	19.46
7345	NE	ARG	B	202	33.985	22.829	1.854	1.00	21.33
7347	CZ	ARG	B	202	34.772	23.882	2.089	1.00	22.51
7348	NH1	ARG	B	202	34.662	24.547	3.222	1.00	23.90
7351	NH2	ARG	B	202	35.663	24.271	1.199	1.00	21.54
7354	C	ARG	B	202	30.517	19.475	1.475	1.00	17.44
7355	O	ARG	B	202	31.179	18.451	1.295	1.00	17.53
7356	N	ALA	B	203	29.804	19.689	2.580	1.00	17.13
7358	CA	ALA	B	203	29.776	18.709	3.658	1.00	16.93
7360	CB	ALA	B	203	28.967	19.200	4.832	1.00	17.56
7364	C	ALA	B	203	29.211	17.389	3.179	1.00	17.03
7365	O	ALA	B	203	29.704	16.351	3.574	1.00	15.70
7366	N	ALA	B	204	28.154	17.439	2.368	1.00	16.79
7368	CA	ALA	B	204	27.548	16.224	1.799	1.00	17.41
7370	CB	ALA	B	204	26.386	16.572	0.915	1.00	17.51
7374	C	ALA	B	204	28.560	15.419	1.002	1.00	17.70
7375	O	ALA	B	204	28.698	14.197	1.200	1.00	17.88
7376	N	VAL	B	205	29.268	16.107	0.109	1.00	17.07
7378	CA	VAL	B	205	30.282	15.471	-0.724	1.00	17.54

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7380	CB	VAL	B	205	30.849	16.429	-1.793	1.00	17.01
7382	CG1	VAL	B	205	31.962	15.769	-2.607	1.00	17.61
7386	CG2	VAL	B	205	29.750	16.884	-2.730	1.00	17.80
7390	C	VAL	B	205	31.400	14.924	0.150	1.00	18.04
7391	O	VAL	B	205	31.802	13.766	-0.005	1.00	17.71
7392	N	ARG	B	206	31.887	15.748	1.078	1.00	18.26
7394	CA	ARG	B	206	32.974	15.348	1.963	1.00	18.54
7396	CB	ARG	B	206	33.393	16.497	2.878	1.00	19.04
7399	CG	ARG	B	206	34.211	17.532	2.179	1.00	18.96
7402	CD	ARG	B	206	34.665	18.637	3.113	1.00	20.46
7405	NE	ARG	B	206	35.712	19.448	2.531	1.00	20.99
7407	CZ	ARG	B	206	36.218	20.545	3.102	1.00	21.01
7408	NH1	ARG	B	206	35.771	20.974	4.275	1.00	20.38
7411	NH2	ARG	B	206	37.190	21.204	2.495	1.00	20.62
7414	C	ARG	B	206	32.582	14.152	2.795	1.00	18.87
7415	O	ARG	B	206	33.368	13.219	2.935	1.00	18.67
7416	N	LEU	B	207	31.346	14.136	3.289	1.00	19.33
7418	CA	LEU	B	207	30.896	13.036	4.141	1.00	20.12
7420	CB	LEU	B	207	29.516	13.310	4.738	1.00	19.99
7423	CG	LEU	B	207	29.431	13.776	6.203	1.00	22.44
7425	CD1	LEU	B	207	30.464	14.770	6.559	1.00	24.69
7429	CD2	LEU	B	207	28.046	14.364	6.440	1.00	24.61
7433	C	LEU	B	207	30.887	11.715	3.370	1.00	20.21
7434	O	LEU	B	207	31.247	10.668	3.922	1.00	20.74
7435	N	GLY	B	208	30.461	11.750	2.110	1.00	20.90
7437	CA	GLY	B	208	30.546	10.578	1.246	1.00	21.11
7440	C	GLY	B	208	31.979	10.097	1.066	1.00	21.83
7441	O	GLY	B	208	32.263	8.898	1.152	1.00	22.91
7442	N	ALA	B	209	32.892	11.029	0.821	1.00	21.98
7444	CA	ALA	B	209	34.292	10.688	0.627	1.00	22.48
7446	CB	ALA	B	209	35.059	11.868	0.052	1.00	22.44
7450	C	ALA	B	209	34.934	10.189	1.928	1.00	23.19
7451	O	ALA	B	209	35.703	9.232	1.906	1.00	23.21
7452	N	LEU	B	210	34.582	10.804	3.058	1.00	23.38
7454	CA	LEU	B	210	35.144	10.429	4.355	1.00	23.77
7456	CB	LEU	B	210	34.733	11.429	5.440	1.00	23.69
7459	CG	LEU	B	210	35.459	12.768	5.355	1.00	23.52
7461	CD1	LEU	B	210	34.830	13.745	6.336	1.00	22.14
7465	CD2	LEU	B	210	36.962	12.569	5.630	1.00	24.32
7469	C	LEU	B	210	34.721	9.031	4.780	1.00	24.42
7470	O	LEU	B	210	35.379	8.410	5.603	1.00	24.38
7471	N	SER	B	211	33.627	8.541	4.211	1.00	25.75
7473	CA	SER	B	211	33.176	7.180	4.458	1.00	26.29
7475	CB	BSER	B	211	31.724	6.990	3.992	0.35	26.33
7476	CB	ASER	B	211	31.733	7.003	3.960	0.65	26.73
7481	OG	BSER	B	211	31.635	6.814	2.589	0.35	25.17
7482	OG	ASER	B	211	30.884	8.043	4.437	0.65	28.22
7485	C	SER	B	211	34.096	6.146	3.779	1.00	26.79
7486	O	SER	B	211	33.943	4.960	4.011	1.00	27.11
7487	N	ALA	B	212	35.052	6.609	2.971	1.00	27.48
7489	CA	ALA	B	212	35.807	5.765	2.045	1.00	28.00
7491	CB	ALA	B	212	35.502	6.200	0.610	1.00	27.64

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7495	C	ALA	B	212	37.330	5.735	2.259	1.00	28.36
7496	O	ALA	B	212	38.075	5.478	1.305	1.00	28.63
7497	N	GLY	B	213	37.793	6.017	3.480	1.00	28.63
7499	CA	GLY	B	213	39.190	5.812	3.848	1.00	28.66
7502	C	GLY	B	213	40.160	6.623	3.013	1.00	29.30
7503	O	GLY	B	213	39.829	7.754	2.628	1.00	29.18
7504	N	ASP	B	214	41.337	6.047	2.725	1.00	29.91
7506	CA	ASP	B	214	42.401	6.716	1.945	1.00	30.40
7508	CB	ASP	B	214	43.629	5.798	1.749	1.00	31.13
7511	CG	ASP	B	214	44.248	5.315	3.055	1.00	32.74
7512	OD1	ASP	B	214	44.060	5.963	4.113	1.00	34.47
7513	OD2	ASP	B	214	44.958	4.280	3.097	1.00	35.20
7514	C	ASP	B	214	41.960	7.157	0.541	1.00	30.05
7515	O	ASP	B	214	42.333	8.224	0.068	1.00	29.72
7516	N	LYS	B	215	41.203	6.319	-0.150	1.00	30.05
7518	CA	LYS	B	215	40.854	6.614	-1.546	1.00	29.92
7520	CB	LYS	B	215	40.230	5.391	-2.199	1.00	30.71
7523	CG	LYS	B	215	40.214	5.394	-3.723	1.00	32.45
7526	CD	LYS	B	215	39.887	3.980	-4.222	1.00	34.64
7529	CE	LYS	B	215	39.790	3.882	-5.732	1.00	36.80
7532	NZ	LYS	B	215	39.315	2.521	-6.190	1.00	38.07
7536	C	LYS	B	215	39.906	7.821	-1.634	1.00	28.89
7537	O	LYS	B	215	40.045	8.661	-2.525	1.00	28.45
7538	N	GLY	B	216	38.972	7.902	-0.689	1.00	27.81
7540	CA	GLY	B	216	38.049	9.018	-0.591	1.00	27.11
7543	C	GLY	B	216	38.781	10.292	-0.243	1.00	26.53
7544	O	GLY	B	216	38.559	11.333	-0.840	1.00	26.52
7545	N	ARG	B	217	39.690	10.198	0.720	1.00	26.28
7547	CA	ARG	B	217	40.519	11.340	1.099	1.00	25.74
7549	CB	ARG	B	217	41.263	11.018	2.393	1.00	25.35
7552	CG	ARG	B	217	40.332	11.005	3.598	1.00	28.38
7555	CD	ARG	B	217	40.945	10.453	4.857	1.00	31.47
7558	NE	ARG	B	217	40.208	10.787	6.078	1.00	33.37
7560	CZ	ARG	B	217	40.258	11.974	6.697	1.00	36.00
7561	NH1	ARG	B	217	40.977	12.979	6.200	1.00	39.28
7564	NH2	ARG	B	217	39.575	12.170	7.810	1.00	34.96
7567	C	ARG	B	217	41.471	11.800	-0.027	1.00	24.69
7568	O	ARG	B	217	41.743	12.983	-0.161	1.00	24.52
7569	N	ARG	B	218	41.956	10.873	-0.844	1.00	24.21
7571	CA	ARG	B	218	42.809	11.210	-1.983	1.00	23.79
7573	CB	ARG	B	218	43.340	9.927	-2.637	1.00	24.37
7576	CG	ARG	B	218	44.257	10.097	-3.872	1.00	27.47
7579	CD	ARG	B	218	43.908	9.115	-5.003	1.00	32.66
7582	NE	ARG	B	218	45.013	8.799	-5.908	1.00	36.58
7584	CZ	ARG	B	218	45.406	9.552	-6.933	1.00	39.40
7585	NH1	ARG	B	218	46.425	9.145	-7.688	1.00	40.57
7588	NH2	ARG	B	218	44.809	10.714	-7.204	1.00	39.74
7591	C	ARG	B	218	42.025	12.047	-3.005	1.00	22.91
7592	O	ARG	B	218	42.599	12.928	-3.640	1.00	22.18
7593	N	ALA	B	219	40.726	11.759	-3.149	1.00	21.70
7595	CA	ALA	B	219	39.845	12.476	-4.066	1.00	21.49
7597	CB	ALA	B	219	38.667	11.618	-4.422	1.00	21.35

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7601	C	ALA	B	219	39.340	13.818	-3.523	1.00	21.64
7602	O	ALA	B	219	38.756	14.587	-4.270	1.00	20.84
7603	N	LEU	B	220	39.563	14.090	-2.240	1.00	21.58
7605	CA	LEU	B	220	39.003	15.285	-1.600	1.00	22.20
7607	CB	LEU	B	220	39.340	15.335	-0.110	1.00	22.43
7610	CG	LEU	B	220	38.407	14.580	0.840	1.00	22.95
7612	CD1	LEU	B	220	38.991	14.642	2.244	1.00	24.14
7616	CD2	LEU	B	220	37.002	15.153	0.810	1.00	24.62
7620	C	LEU	B	220	39.364	16.616	-2.239	1.00	21.85
7621	O	LEU	B	220	38.482	17.438	-2.393	1.00	22.54
7622	N	PRO	B	221	40.627	16.872	-2.583	1.00	22.19
7623	CA	PRO	B	221	40.969	18.150	-3.227	1.00	22.28
7625	CB	PRO	B	221	42.442	17.987	-3.589	1.00	22.39
7628	CG	PRO	B	221	42.951	16.960	-2.616	1.00	23.34
7631	CD	PRO	B	221	41.812	16.025	-2.379	1.00	22.27
7634	C	PRO	B	221	40.115	18.420	-4.460	1.00	21.79
7635	O	PRO	B	221	39.580	19.513	-4.592	1.00	21.54
7636	N	VAL	B	222	39.945	17.431	-5.331	1.00	21.34
7638	CA	VAL	B	222	39.131	17.616	-6.533	1.00	20.96
7640	CB	VAL	B	222	39.431	16.533	-7.601	1.00	21.09
7642	CG1	VAL	B	222	38.492	16.664	-8.787	1.00	20.79
7646	CG2	VAL	B	222	40.885	16.668	-8.085	1.00	22.50
7650	C	VAL	B	222	37.620	17.635	-6.214	1.00	20.48
7651	O	VAL	B	222	36.877	18.411	-6.804	1.00	20.29
7652	N	LEU	B	223	37.172	16.773	-5.307	1.00	20.17
7654	CA	LEU	B	223	35.750	16.717	-4.924	1.00	19.91
7656	CB	LEU	B	223	35.466	15.562	-3.957	1.00	20.52
7659	CG	LEU	B	223	35.293	14.173	-4.587	1.00	21.95
7661	CD1	LEU	B	223	35.296	13.095	-3.512	1.00	22.04
7665	CD2	LEU	B	223	34.039	14.111	-5.407	1.00	23.07
7669	C	LEU	B	223	35.327	18.015	-4.253	1.00	19.72
7670	O	LEU	B	223	34.188	18.456	-4.381	1.00	19.07
7671	N	ASP	B	224	36.250	18.599	-3.503	1.00	19.68
7673	CA	ASP	B	224	36.042	19.893	-2.883	1.00	19.94
7675	CB	ASP	B	224	37.272	20.287	-2.069	1.00	19.86
7678	CG	ASP	B	224	37.289	19.671	-0.705	1.00	22.67
7679	OD1	ASP	B	224	36.256	19.094	-0.288	1.00	23.35
7680	OD2	ASP	B	224	38.304	19.744	0.036	1.00	25.14
7681	C	ASP	B	224	35.778	20.972	-3.908	1.00	19.81
7682	O	ASP	B	224	34.910	21.795	-3.702	1.00	19.95
7683	N	LYS	B	225	36.541	20.990	-4.996	1.00	19.94
7685	CA	LYS	B	225	36.368	22.027	-6.013	1.00	20.31
7687	CB	LYS	B	225	37.525	22.048	-7.022	1.00	20.63
7690	CG	LYS	B	225	38.973	22.184	-6.439	1.00	22.72
7693	CD	BLYS	B	225	39.100	23.053	-5.155	0.35	21.46
7694	CD	ALYS	B	225	39.001	22.753	-5.014	0.65	25.09
7699	CE	BLYS	B	225	39.223	22.270	-3.837	0.35	19.92
7700	CE	ALYS	B	225	39.871	23.974	-4.801	0.65	25.51
7705	NZ	BLYS	B	225	40.570	21.728	-3.502	0.35	14.63
7706	NZ	ALYS	B	225	39.377	24.575	-3.546	0.65	24.29
7713	C	LYS	B	225	35.049	21.804	-6.718	1.00	19.81
7714	O	LYS	B	225	34.320	22.762	-6.982	1.00	19.64

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7715	N	TYR	B	226	34.733	20.536	-6.979	1.00	19.10
7717	CA	TYR	B	226	33.437	20.151	-7.525	1.00	18.47
7719	CB	TYR	B	226	33.307	18.624	-7.646	1.00	18.62
7722	CG	TYR	B	226	31.883	18.168	-7.875	1.00	17.81
7723	CD1	TYR	B	226	31.300	18.256	-9.132	1.00	17.52
7725	CE1	TYR	B	226	29.994	17.859	-9.337	1.00	20.05
7727	CZ	TYR	B	226	29.232	17.374	-8.279	1.00	18.47
7728	OH	TYR	B	226	27.919	16.982	-8.500	1.00	17.52
7730	CE2	TYR	B	226	29.785	17.299	-7.026	1.00	17.57
7732	CD2	TYR	B	226	31.112	17.694	-6.829	1.00	17.49
7734	C	TYR	B	226	32.331	20.699	-6.643	1.00	18.41
7735	O	TYR	B	226	31.452	21.411	-7.122	1.00	18.11
7736	N	ALA	B	227	32.417	20.408	-5.345	1.00	18.13
7738	CA	ALA	B	227	31.403	20.799	-4.377	1.00	18.18
7740	CB	ALA	B	227	31.723	20.221	-3.021	1.00	17.94
7744	C	ALA	B	227	31.281	22.316	-4.251	1.00	18.61
7745	O	ALA	B	227	30.196	22.851	-4.063	1.00	18.11
7746	N	GLU	B	228	32.407	22.996	-4.328	1.00	19.06
7748	CA	GLU	B	228	32.418	24.439	-4.177	1.00	20.24
7750	CB	GLU	B	228	33.864	24.949	-4.123	1.00	20.64
7753	CG	GLU	B	228	34.451	24.809	-2.730	1.00	23.29
7756	CD	GLU	B	228	35.947	24.586	-2.731	1.00	26.70
7757	OE1	GLU	B	228	36.464	23.942	-1.768	1.00	29.92
7758	OE2	GLU	B	228	36.592	25.044	-3.686	1.00	27.85
7759	C	GLU	B	228	31.636	25.080	-5.300	1.00	20.03
7760	O	GLU	B	228	30.842	25.982	-5.063	1.00	20.42
7761	N	SER	B	229	31.824	24.584	-6.521	1.00	20.10
7763	CA	SER	B	229	31.140	25.146	-7.663	1.00	20.21
7765	CB	SER	B	229	31.838	24.755	-8.958	1.00	20.74
7768	OG	SER	B	229	33.134	25.319	-8.986	1.00	21.81
7770	C	SER	B	229	29.655	24.795	-7.704	1.00	19.69
7771	O	SER	B	229	28.845	25.675	-7.972	1.00	19.58
7772	N	ILE	B	230	29.283	23.538	-7.451	1.00	19.26
7774	CA	ILE	B	230	27.855	23.173	-7.467	1.00	19.00
7776	CB	ILE	B	230	27.588	21.634	-7.493	1.00	19.39
7778	CG1	ILE	B	230	28.132	20.922	-6.249	1.00	19.42
7781	CD1	ILE	B	230	27.348	19.661	-5.883	1.00	19.21
7785	CG2	ILE	B	230	28.145	20.996	-8.778	1.00	20.74
7789	C	ILE	B	230	27.118	23.798	-6.292	1.00	18.75
7790	O	ILE	B	230	25.934	24.062	-6.404	1.00	18.69
7791	N	GLY	B	231	27.825	24.000	-5.179	1.00	17.92
7793	CA	GLY	B	231	27.260	24.588	-3.977	1.00	18.54
7796	C	GLY	B	231	26.885	26.044	-4.189	1.00	18.41
7797	O	GLY	B	231	25.776	26.467	-3.838	1.00	18.39
7798	N	LEU	B	232	27.791	26.809	-4.801	1.00	18.03
7800	CA	LEU	B	232	27.463	28.191	-5.176	1.00	17.92
7802	CB	LEU	B	232	28.697	28.973	-5.644	1.00	17.76
7805	CG	LEU	B	232	28.471	30.416	-6.137	1.00	18.58
7807	CD1	LEU	B	232	27.676	31.245	-5.123	1.00	20.10
7811	CD2	LEU	B	232	29.783	31.085	-6.471	1.00	19.77
7815	C	LEU	B	232	26.371	28.184	-6.232	1.00	17.69
7816	O	LEU	B	232	25.391	28.929	-6.125	1.00	17.69

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7817	N	ALA	B	233	26.520	27.332	-7.243	1.00	17.54
7819	CA	ALA	B	233	25.535	27.255	-8.330	1.00	17.52
7821	CB	ALA	B	233	25.937	26.175	-9.322	1.00	17.72
7825	C	ALA	B	233	24.133	26.996	-7.801	1.00	16.87
7826	O	ALA	B	233	23.149	27.503	-8.321	1.00	16.72
7827	N	PHE	B	234	24.055	26.207	-6.738	1.00	17.20
7829	CA	PHE	B	234	22.796	25.770	-6.175	1.00	17.20
7831	CB	PHE	B	234	23.077	24.798	-5.020	1.00	17.86
7834	CG	PHE	B	234	21.913	23.952	-4.635	1.00	19.19
7835	CD1	PHE	B	234	21.908	22.595	-4.939	1.00	23.96
7837	CE1	PHE	B	234	20.833	21.786	-4.576	1.00	25.08
7839	CZ	PHE	B	234	19.753	22.346	-3.895	1.00	23.44
7841	CE2	PHE	B	234	19.766	23.705	-3.578	1.00	21.13
7843	CD2	PHE	B	234	20.837	24.489	-3.936	1.00	19.81
7845	C	PHE	B	234	22.023	26.972	-5.659	1.00	17.12
7846	O	PHE	B	234	20.817	27.075	-5.856	1.00	16.09
7847	N	GLN	B	235	22.724	27.860	-4.969	1.00	16.71
7849	CA	GLN	B	235	22.093	29.040	-4.427	1.00	17.18
7851	CB	GLN	B	235	22.918	29.661	-3.304	1.00	16.88
7854	CG	GLN	B	235	22.173	30.781	-2.566	1.00	16.78
7857	CD	GLN	B	235	20.856	30.332	-1.970	1.00	18.18
7858	OE1	GLN	B	235	20.783	29.271	-1.353	1.00	17.96
7859	NE2	GLN	B	235	19.818	31.140	-2.138	1.00	15.32
7862	C	GLN	B	235	21.821	30.089	-5.501	1.00	16.98
7863	O	GLN	B	235	20.842	30.800	-5.392	1.00	16.15
7864	N	VAL	B	236	22.640	30.184	-6.544	1.00	17.46
7866	CA	VAL	B	236	22.265	31.160	-7.590	1.00	18.23
7868	CB	VAL	B	236	23.405	31.708	-8.547	1.00	18.68
7870	CG1	VAL	B	236	24.747	31.119	-8.271	1.00	19.87
7874	CG2	VAL	B	236	23.019	31.733	-10.030	1.00	19.70
7878	C	VAL	B	236	21.003	30.665	-8.279	1.00	17.45
7879	O	VAL	B	236	20.139	31.457	-8.531	1.00	17.04
7880	N	GLN	B	237	20.856	29.350	-8.447	1.00	17.88
7882	CA	GLN	B	237	19.649	28.785	-9.035	1.00	18.28
7884	CB	GLN	B	237	19.783	27.288	-9.337	1.00	18.86
7887	CG	GLN	B	237	18.561	26.715	-10.056	1.00	20.61
7890	CD	GLN	B	237	18.402	27.211	-11.478	1.00	23.91
7891	OE1	GLN	B	237	19.207	27.995	-11.962	1.00	27.71
7892	NE2	GLN	B	237	17.361	26.738	-12.157	1.00	25.53
7895	C	GLN	B	237	18.469	29.005	-8.135	1.00	17.68
7896	O	GLN	B	237	17.381	29.326	-8.612	1.00	18.18
7897	N	ASP	B	238	18.673	28.830	-6.832	1.00	16.95
7899	CA	ASP	B	238	17.624	29.133	-5.872	1.00	16.59
7901	CB	ASP	B	238	18.084	28.803	-4.452	1.00	15.86
7904	CG	ASP	B	238	16.988	28.976	-3.451	1.00	16.32
7905	OD1	ASP	B	238	16.037	28.162	-3.445	1.00	17.49
7906	OD2	ASP	B	238	16.959	29.929	-2.651	1.00	18.97
7907	C	ASP	B	238	17.186	30.610	-5.985	1.00	16.34
7908	O	ASP	B	238	16.001	30.905	-5.932	1.00	15.59
7909	N	ASP	B	239	18.135	31.526	-6.146	1.00	17.76
7911	CA	ASP	B	239	17.799	32.959	-6.321	1.00	18.83
7913	CB	ASP	B	239	19.044	33.819	-6.384	1.00	19.28

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
7916	CG	ASP	B	239	19.766	33.928	-5.070	1.00	19.95
7917	OD1	ASP	B	239	19.251	33.447	-4.018	1.00	23.46
7918	OD2	ASP	B	239	20.886	34.480	-5.016	1.00	19.63
7919	C	ASP	B	239	17.021	33.192	-7.610	1.00	19.87
7920	O	ASP	B	239	16.020	33.917	-7.629	1.00	20.25
7921	N	ILE	B	240	17.492	32.570	-8.687	1.00	19.96
7923	CA	ILE	B	240	16.845	32.676	-9.986	1.00	20.61
7925	CB	ILE	B	240	17.647	31.902	-11.039	1.00	20.77
7927	CG1	ILE	B	240	18.945	32.645	-11.363	1.00	20.81
7930	CD1	ILE	B	240	19.974	31.792	-11.997	1.00	21.71
7934	CG2	ILE	B	240	16.821	31.682	-12.304	1.00	21.31
7938	C	ILE	B	240	15.413	32.161	-9.932	1.00	20.80
7939	O	ILE	B	240	14.506	32.784	-10.482	1.00	20.05
7940	N	LEU	B	241	15.214	31.014	-9.283	1.00	21.23
7942	CA	LEU	B	241	13.904	30.394	-9.206	1.00	21.82
7944	CB	LEU	B	241	14.009	28.986	-8.620	1.00	22.08
7947	CG	LEU	B	241	14.569	27.953	-9.600	1.00	23.04
7949	CD1	LEU	B	241	14.635	26.592	-8.926	1.00	25.03
7953	CD2	LEU	B	241	13.740	27.874	-10.869	1.00	23.91
7957	C	LEU	B	241	12.955	31.226	-8.384	1.00	22.17
7958	O	LEU	B	241	11.759	31.219	-8.613	1.00	22.86
7959	N	ASP	B	242	13.487	31.928	-7.401	1.00	22.89
7961	CA	ASP	B	242	12.680	32.816	-6.597	1.00	23.68
7963	CB	ASP	B	242	13.538	33.476	-5.526	1.00	24.26
7966	CG	ASP	B	242	12.782	33.732	-4.261	1.00	26.59
7967	OD1	ASP	B	242	12.339	34.885	-4.081	1.00	29.09
7968	OD2	ASP	B	242	12.586	32.842	-3.395	1.00	30.35
7969	C	ASP	B	242	12.018	33.889	-7.468	1.00	24.03
7970	O	ASP	B	242	10.872	34.264	-7.225	1.00	23.75
7971	N	VAL	B	243	12.722	34.380	-8.478	1.00	24.22
7973	CA	VAL	B	243	12.133	35.431	-9.334	1.00	25.09
7975	CB	BVAL	B	243	13.207	36.455	-9.871	0.35	24.92
7976	CB	AVAL	B	243	13.180	36.479	-9.849	0.65	25.18
7979	CG1BVAL	B	243		14.454	35.767	-10.368	0.35	24.74
7980	CG1AVAL	B	243		14.270	36.727	-8.817	0.65	24.27
7987	CG2BVAL	B	243		12.633	37.361	-10.975	0.35	23.96
7988	CG2AVAL	B	243		13.775	36.088	-11.166	0.65	25.87
7995	C	VAL	B	243	11.271	34.851	-10.474	1.00	25.74
7996	O	VAL	B	243	10.167	35.330	-10.688	1.00	25.89
7997	N	VAL	B	244	11.745	33.812	-11.160	1.00	26.96
7999	CA	VAL	B	244	11.065	33.282	-12.350	1.00	27.89
8001	CB	VAL	B	244	12.069	32.914	-13.472	1.00	28.15
8003	CG1	VAL	B	244	12.996	34.083	-13.769	1.00	29.48
8007	CG2	VAL	B	244	12.852	31.642	-13.143	1.00	28.31
8011	C	VAL	B	244	10.158	32.066	-12.136	1.00	28.41
8012	O	VAL	B	244	9.330	31.776	-12.983	1.00	28.51
8013	N	GLY	B	245	10.331	31.335	-11.038	1.00	29.07
8015	CA	GLY	B	245	9.583	30.107	-10.813	1.00	29.72
8018	C	GLY	B	245	8.131	30.378	-10.460	1.00	30.36
8019	O	GLY	B	245	7.793	31.482	-10.070	1.00	31.39
8020	N	ASP	B	246	7.276	29.376	-10.613	1.00	30.83
8022	CA	ASP	B	246	5.885	29.465	-10.194	1.00	31.66

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8024	CB	ASP	B	246	4.996	28.632	-11.128	1.00	32.32
8027	CG	ASP	B	246	3.527	29.006	-11.027	1.00	35.80
8028	OD1	ASP	B	246	2.981	29.516	-12.041	1.00	41.36
8029	OD2	ASP	B	246	2.818	28.820	-9.997	1.00	39.19
8030	C	ASP	B	246	5.782	28.894	-8.790	1.00	30.65
8031	O	ASP	B	246	6.321	27.842	-8.546	1.00	30.56
8032	N	THR	B	247	5.072	29.572	-7.892	1.00	29.92
8034	CA	THR	B	247	4.846	29.080	-6.533	1.00	29.76
8036	CB	THR	B	247	3.814	29.975	-5.811	1.00	29.87
8038	OG1	THR	B	247	4.378	31.272	-5.593	1.00	31.54
8040	CG2	THR	B	247	3.502	29.459	-4.399	1.00	30.40
8044	C	THR	B	247	4.401	27.611	-6.492	1.00	28.88
8045	O	THR	B	247	4.911	26.844	-5.685	1.00	28.30
8046	N	ALA	B	248	3.465	27.222	-7.358	1.00	28.23
8048	CA	ALA	B	248	2.932	25.852	-7.367	1.00	28.33
8050	CB	ALA	B	248	1.809	25.708	-8.391	1.00	28.17
8054	C	ALA	B	248	4.007	24.805	-7.644	1.00	28.26
8055	O	ALA	B	248	3.925	23.687	-7.143	1.00	28.69
8056	N	THR	B	249	4.985	25.172	-8.466	1.00	27.77
8058	CA	THR	B	249	6.091	24.292	-8.824	1.00	27.75
8060	CB	THR	B	249	6.638	24.726	-10.188	1.00	27.90
8062	OG1	THR	B	249	5.596	24.624	-11.164	1.00	30.21
8064	CG2	THR	B	249	7.706	23.767	-10.678	1.00	28.58
8068	C	THR	B	249	7.223	24.275	-7.773	1.00	26.85
8069	O	THR	B	249	7.671	23.202	-7.356	1.00	26.31
8070	N	LEU	B	250	7.654	25.463	-7.348	1.00	25.98
8072	CA	LEU	B	250	8.706	25.627	-6.328	1.00	25.67
8074	CB	LEU	B	250	8.994	27.116	-6.091	1.00	25.92
8077	CG	LEU	B	250	9.408	28.030	-7.239	1.00	27.52
8079	CD1	LEU	B	250	9.656	29.433	-6.691	1.00	27.93
8083	CD2	LEU	B	250	10.625	27.516	-7.954	1.00	28.70
8087	C	LEU	B	250	8.359	25.039	-4.965	1.00	24.61
8088	O	LEU	B	250	9.244	24.625	-4.217	1.00	22.99
8089	N	GLY	B	251	7.077	25.078	-4.612	1.00	23.96
8091	CA	GLY	B	251	6.636	24.759	-3.265	1.00	23.66
8094	C	GLY	B	251	6.808	25.892	-2.263	1.00	23.66
8095	O	GLY	B	251	6.449	25.748	-1.105	1.00	23.25
8096	N	LYS	B	252	7.310	27.036	-2.721	1.00	23.45
8098	CA	LYS	B	252	7.499	28.207	-1.881	1.00	23.55
8100	CB	LYS	B	252	8.913	28.217	-1.262	1.00	23.19
8103	CG	LYS	B	252	10.065	28.100	-2.279	1.00	22.81
8106	CD	LYS	B	252	11.443	27.892	-1.587	1.00	21.30
8109	CE	LYS	B	252	12.575	28.125	-2.537	1.00	19.95
8112	NZ	LYS	B	252	13.876	27.549	-2.087	1.00	18.06
8116	C	LYS	B	252	7.248	29.466	-2.729	1.00	24.42
8117	O	LYS	B	252	7.280	29.414	-3.961	1.00	24.38
8118	N	ARG	B	253	7.024	30.592	-2.066	1.00	25.44
8120	CA	ARG	B	253	6.534	31.795	-2.744	1.00	26.73
8122	CB	ARG	B	253	6.006	32.830	-1.737	1.00	27.67
8125	CG	ARG	B	253	4.510	33.101	-1.907	1.00	31.24
8128	CD	ARG	B	253	3.825	33.710	-0.700	1.00	35.52
8131	NE	ARG	B	253	3.150	32.704	0.116	1.00	37.39

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8133	CZ	ARG	B	253	2.036	32.056	-0.235	1.00	39.88
8134	NH1	ARG	B	253	1.451	32.263	-1.417	1.00	41.43
8137	NH2	ARG	B	253	1.518	31.167	0.605	1.00	41.57
8140	C	ARG	B	253	7.550	32.432	-3.685	1.00	25.93
8141	O	ARG	B	253	8.642	32.852	-3.283	1.00	25.79
8142	N	GLN	B	254	7.176	32.480	-4.955	1.00	25.68
8144	CA	GLN	B	254	7.848	33.323	-5.931	1.00	25.41
8146	CB	GLN	B	254	7.076	33.337	-7.255	1.00	25.85
8149	CG	BGLN	B	254	7.707	34.187	-8.363	0.35	25.46
8150	CG	AGLN	B	254	7.696	34.266	-8.323	0.65	26.52
8155	CD	BGLN	B	254	7.388	35.665	-8.261	0.35	25.75
8156	CD	AGLN	B	254	6.858	34.376	-9.595	0.65	29.40
8157	OE1BGLN	B	254		8.227	36.501	-8.593	0.35	26.04
8158	OE1AGLN	B	254		7.335	34.901	-10.609	0.65	30.77
8159	NE2BGLN	B	254		6.180	35.993	-7.809	0.35	25.98
8160	NE2AGLN	B	254		5.622	33.888	-9.547	0.65	29.10
8165	C	GLN	B	254	7.900	34.730	-5.369	1.00	24.67
8166	O	GLN	B	254	6.942	35.184	-4.755	1.00	24.03
8167	N	GLY	B	255	9.023	35.413	-5.565	1.00	24.23
8169	CA	GLY	B	255	9.107	36.829	-5.264	1.00	24.15
8172	C	GLY	B	255	9.417	37.151	-3.816	1.00	24.34
8173	O	GLY	B	255	9.464	38.307	-3.465	1.00	24.07
8174	N	ALA	B	256	9.656	36.142	-2.983	1.00	24.66
8176	CA	ALA	B	256	9.909	36.359	-1.559	1.00	25.08
8178	CB	ALA	B	256	9.978	35.024	-0.833	1.00	24.93
8182	C	ALA	B	256	11.179	37.180	-1.288	1.00	25.56
8183	O	ALA	B	256	11.213	37.979	-0.353	1.00	26.42
8184	N	ASP	B	257	12.210	37.000	-2.105	1.00	25.88
8186	CA	ASP	B	257	13.466	37.739	-1.932	1.00	26.25
8188	CB	ASP	B	257	14.564	37.191	-2.848	1.00	26.11
8191	CG	ASP	B	257	15.025	35.791	-2.463	1.00	26.45
8192	OD1	ASP	B	257	14.815	35.353	-1.299	1.00	26.12
8193	OD2	ASP	B	257	15.602	35.054	-3.292	1.00	25.40
8194	C	ASP	B	257	13.286	39.221	-2.241	1.00	27.05
8195	O	ASP	B	257	13.823	40.074	-1.549	1.00	26.45
8196	N	GLN	B	258	12.545	39.520	-3.304	1.00	28.65
8198	CA	GLN	B	258	12.278	40.908	-3.691	1.00	29.67
8200	CB	BGLN	B	258	11.590	40.972	-5.061	0.35	29.64
8201	CB	AGLN	B	258	11.557	40.939	-5.046	0.65	30.10
8206	CG	BGLN	B	258	12.546	40.710	-6.226	0.35	29.64
8207	CG	AGLN	B	258	11.357	42.333	-5.625	0.65	31.67
8212	CD	BGLN	B	258	11.961	41.060	-7.589	0.35	29.88
8213	CD	AGLN	B	258	9.896	42.666	-5.883	0.65	33.37
8214	OE1BGLN	B	258		12.242	40.380	-8.581	0.35	29.18
8215	OE1AGLN	B	258		9.502	42.893	-7.025	0.65	34.64
8216	NE2BGLN	B	258		11.163	42.126	-7.646	0.35	29.79
8217	NE2AGLN	B	258		9.094	42.705	-4.820	0.65	34.91
8222	C	GLN	B	258	11.455	41.638	-2.614	1.00	29.97
8223	O	GLN	B	258	11.755	42.780	-2.274	1.00	29.34
8224	N	GLN	B	259	10.439	40.957	-2.080	1.00	30.70
8226	CA	GLN	B	259	9.658	41.427	-0.922	1.00	31.61
8228	CB	GLN	B	259	8.769	40.285	-0.410	1.00	32.41

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8231	CG	GLN	B	259	7.466	40.703	0.244	1.00	35.31
8234	CD	GLN	B	259	6.317	40.769	-0.744	1.00	39.68
8235	OE1	GLN	B	259	5.925	41.861	-1.174	1.00	43.25
8236	NE2	GLN	B	259	5.780	39.605	-1.119	1.00	42.40
8239	C	GLN	B	259	10.546	41.934	0.242	1.00	31.29
8240	O	GLN	B	259	10.321	43.032	0.776	1.00	31.47
8241	N	LEU	B	260	11.552	41.135	0.612	1.00	30.18
8243	CA	LEU	B	260	12.421	41.420	1.761	1.00	29.88
8245	CB	LEU	B	260	12.851	40.109	2.446	1.00	29.79
8248	CG	LEU	B	260	11.792	39.268	3.160	1.00	30.18
8250	CD1	LEU	B	260	12.453	38.363	4.192	1.00	29.62
8254	CD2	LEU	B	260	10.742	40.140	3.817	1.00	31.47
8258	C	LEU	B	260	13.681	42.207	1.413	1.00	28.94
8259	O	LEU	B	260	14.431	42.593	2.307	1.00	29.69
8260	N	GLY	B	261	13.921	42.429	0.128	1.00	27.95
8262	CA	GLY	B	261	15.133	43.084	-0.333	1.00	26.93
8265	C	GLY	B	261	16.398	42.279	-0.094	1.00	25.88
8266	O	GLY	B	261	17.436	42.845	0.261	1.00	25.61
8267	N	LYS	B	262	16.325	40.959	-0.277	1.00	24.82
8269	CA	LYS	B	262	17.501	40.115	-0.136	1.00	23.75
8271	CB	LYS	B	262	17.153	38.627	-0.295	1.00	23.56
8274	CG	LYS	B	262	16.230	38.069	0.762	1.00	23.25
8277	CD	LYS	B	262	16.916	37.862	2.096	1.00	21.56
8280	CE	LYS	B	262	15.901	37.433	3.158	1.00	23.14
8283	NZ	LYS	B	262	16.536	37.070	4.482	1.00	21.85
8287	C	LYS	B	262	18.515	40.497	-1.195	1.00	23.58
8288	O	LYS	B	262	18.145	40.845	-2.337	1.00	23.29
8289	N	SER	B	263	19.785	40.474	-0.803	1.00	22.82
8291	CA	SER	B	263	20.885	40.514	-1.746	1.00	22.51
8293	CB	SER	B	263	22.206	40.785	-1.035	1.00	22.93
8296	OG	SER	B	263	22.263	42.141	-0.613	1.00	23.10
8298	C	SER	B	263	20.934	39.170	-2.452	1.00	22.79
8299	O	SER	B	263	21.051	38.122	-1.784	1.00	22.61
8300	N	THR	B	264	20.786	39.194	-3.782	1.00	21.90
8302	CA	THR	B	264	20.764	37.973	-4.593	1.00	22.01
8304	CB	THR	B	264	19.304	37.496	-4.909	1.00	22.17
8306	OG1	THR	B	264	18.667	38.392	-5.827	1.00	23.42
8308	CG2	THR	B	264	18.386	37.525	-3.707	1.00	21.68
8312	C	THR	B	264	21.499	38.175	-5.908	1.00	21.99
8313	O	THR	B	264	21.731	39.306	-6.354	1.00	21.16
8314	N	TYR	B	265	21.841	37.066	-6.553	1.00	21.84
8316	CA	TYR	B	265	22.470	37.134	-7.864	1.00	22.04
8318	CB	TYR	B	265	22.959	35.754	-8.319	1.00	21.34
8321	CG	TYR	B	265	24.340	35.435	-7.803	1.00	20.33
8322	CD1	TYR	B	265	25.430	35.422	-8.654	1.00	20.38
8324	CE1	TYR	B	265	26.686	35.129	-8.197	1.00	20.95
8326	CZ	TYR	B	265	26.877	34.859	-6.866	1.00	20.10
8327	OH	TYR	B	265	28.142	34.576	-6.417	1.00	24.40
8329	CE2	TYR	B	265	25.818	34.876	-5.989	1.00	19.89
8331	CD2	TYR	B	265	24.561	35.161	-6.455	1.00	18.52
8333	C	TYR	B	265	21.588	37.816	-8.933	1.00	22.40
8334	O	TYR	B	265	22.075	38.711	-9.612	1.00	22.20

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8335	N	PRO	B	266	20.328	37.413	-9.102	1.00	22.68
8336	CA	PRO	B	266	19.448	38.083	-10.073	1.00	23.28
8338	CB	PRO	B	266	18.131	37.309	-9.984	1.00	23.44
8341	CG	PRO	B	266	18.438	36.064	-9.253	1.00	23.26
8344	CD	PRO	B	266	19.635	36.319	-8.412	1.00	23.08
8347	C	PRO	B	266	19.193	39.550	-9.744	1.00	23.45
8348	O	PRO	B	266	19.084	40.350	-10.668	1.00	23.18
8349	N	ALA	B	267	19.099	39.890	-8.460	1.00	23.47
8351	CA	ALA	B	267	18.821	41.268	-8.062	1.00	23.58
8353	CB	ALA	B	267	18.569	41.386	-6.560	1.00	23.84
8357	C'	ALA	B	267	19.962	42.155	-8.483	1.00	23.82
8358	O	ALA	B	267	19.742	43.216	-9.062	1.00	24.38
8359	N	LEU	B	268	21.184	41.692	-8.247	1.00	23.53
8361	CA	LEU	B	268	22.375	42.447	-8.586	1.00	23.59
8363	CB	LEU	B	268	23.566	41.908	-7.798	1.00	23.51
8366	CG	LEU	B	268	24.934	42.511	-8.113	1.00	23.92
8368	CD1	LEU	B	268	24.947	44.021	-7.830	1.00	24.92
8372	CD2	LEU	B	268	26.012	41.800	-7.318	1.00	24.12
8376	C	LEU	B	268	22.704	42.437	-10.082	1.00	23.25
8377	O	LEU	B	268	22.964	43.479	-10.664	1.00	23.31
8378	N	LEU	B	269	22.693	41.253	-10.683	1.00	22.76
8380	CA	LEU	B	269	23.281	41.018	-11.995	1.00	22.56
8382	CB	LEU	B	269	24.093	39.726	-11.983	1.00	22.53
8385	CG	LEU	B	269	25.314	39.686	-11.062	1.00	24.16
8387	CD1	LEU	B	269	25.881	38.277	-11.022	1.00	25.08
8391	CD2	LEU	B	269	26.394	40.674	-11.518	1.00	25.88
8395	C	LEU	B	269	22.237	40.925	-13.089	1.00	21.93
8396	O	LEU	B	269	22.567	40.925	-14.273	1.00	21.98
8397	N	GLY	B	270	20.981	40.880	-12.696	1.00	21.10
8399	CA	GLY	B	270	19.925	40.537	-13.619	1.00	21.48
8402	C	GLY	B	270	19.923	39.035	-13.860	1.00	21.79
8403	O	GLY	B	270	20.883	38.320	-13.530	1.00	20.41
8404	N	LEU	B	271	18.831	38.570	-14.445	1.00	22.27
8406	CA	LEU	B	271	18.587	37.145	-14.645	1.00	23.11
8408	CB	LEU	B	271	17.169	36.923	-15.161	1.00	23.57
8411	CG	LEU	B	271	16.145	36.966	-14.051	1.00	23.96
8413	CD1	LEU	B	271	14.712	36.988	-14.638	1.00	25.68
8417	CD2	LEU	B	271	16.375	35.748	-13.152	1.00	24.82
8421	C	LEU	B	271	19.554	36.493	-15.601	1.00	23.62
8422	O	LEU	B	271	19.999	35.393	-15.348	1.00	22.96
8423	N	GLU	B	272	19.885	37.158	-16.704	1.00	24.28
8425	CA	GLU	B	272	20.703	36.498	-17.715	1.00	25.35
8427	CB	GLU	B	272	20.712	37.237	-19.049	1.00	26.22
8430	CG	GLU	B	272	21.247	36.373	-20.184	1.00	30.72
8433	CD	GLU	B	272	20.177	35.523	-20.858	1.00	36.13
8434	OE1	GLU	B	272	19.801	35.857	-22.020	1.00	40.61
8435	OE2	GLU	B	272	19.725	34.513	-20.244	1.00	38.13
8436	C	GLU	B	272	22.116	36.293	-17.220	1.00	24.46
8437	O	GLU	B	272	22.658	35.215	-17.405	1.00	23.99
8438	N	GLN	B	273	22.707	37.305	-16.582	1.00	23.54
8440	CA	GLN	B	273	24.052	37.148	-16.019	1.00	23.89
8442	CB	GLN	B	273	24.640	38.488	-15.569	1.00	23.95

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8445	CG	GLN	B	273	25.057	39.407	-16.701	1.00	26.62
8448	CD	GLN	B	273	25.436	40.804	-16.197	1.00	29.62
8449	OE1	GLN	B	273	26.041	40.939	-15.140	1.00	29.56
8450	NE2	GLN	B	273	25.046	41.834	-16.941	1.00	32.63
8453	C	GLN	B	273	24.042	36.157	-14.848	1.00	23.16
8454	O	GLN	B	273	24.994	35.428	-14.656	1.00	23.94
8455	N	ALA	B	274	22.968	36.130	-14.071	1.00	22.86
8457	CA	ALA	B	274	22.852	35.161	-12.985	1.00	22.78
8459	CB	ALA	B	274	21.591	35.413	-12.169	1.00	22.56
8463	C	ALA	B	274	22.848	33.738	-13.565	1.00	22.60
8464	O	ALA	B	274	23.542	32.873	-13.071	1.00	22.64
8465	N	ARG	B	275	22.085	33.520	-14.632	1.00	22.89
8467	CA	ARG	B	275	22.048	32.213	-15.299	1.00	23.30
8469	CB	ARG	B	275	21.012	32.205	-16.431	1.00	23.67
8472	CG	ARG	B	275	19.594	32.090	-15.944	1.00	25.28
8475	CD	ARG	B	275	18.542	32.199	-17.031	1.00	27.92
8478	NE	ARG	B	275	17.209	31.888	-16.503	1.00	30.36
8480	CZ	ARG	B	275	16.104	32.616	-16.697	1.00	32.35
8481	NH1	ARG	B	275	16.121	33.727	-17.423	1.00	31.95
8484	NH2	ARG	B	275	14.954	32.217	-16.160	1.00	34.03
8487	C	ARG	B	275	23.424	31.827	-15.854	1.00	23.20
8488	O	ARG	B	275	23.843	30.669	-15.783	1.00	22.27
8489	N	LYS	B	276	24.111	32.807	-16.421	1.00	23.01
8491	CA	LYS	B	276	25.418	32.595	-16.998	1.00	22.90
8493	CB	LYS	B	276	25.870	33.833	-17.774	1.00	23.16
8496	CG	LYS	B	276	27.307	33.794	-18.251	1.00	24.89
8499	CD	LYS	B	276	27.542	32.619	-19.190	1.00	28.29
8502	CE	LYS	B	276	28.672	32.892	-20.166	1.00	29.58
8505	NZ	LYS	B	276	29.948	33.113	-19.451	1.00	30.99
8509	C	LYS	B	276	26.422	32.253	-15.893	1.00	22.40
8510	O	LYS	B	276	27.270	31.400	-16.086	1.00	22.05
8511	N	LYS	B	277	26.312	32.901	-14.742	1.00	21.92
8513	CA	LYS	B	277	27.191	32.604	-13.612	1.00	22.26
8515	CB	LYS	B	277	26.959	33.566	-12.444	1.00	22.86
8518	CG	LYS	B	277	27.325	35.029	-12.759	1.00	26.57
8521	CD	LYS	B	277	28.574	35.530	-12.019	1.00	30.08
8524	CE	LYS	B	277	29.067	36.885	-12.583	1.00	31.95
8527	NZ	LYS	B	277	30.540	37.060	-12.449	1.00	33.10
8531	C	LYS	B	277	26.982	31.151	-13.175	1.00	21.47
8532	O	LYS	B	277	27.939	30.422	-12.944	1.00	21.43
8533	N	ALA	B	278	25.725	30.729	-13.101	1.00	20.57
8535	CA	ALA	B	278	25.408	29.366	-12.697	1.00	20.64
8537	CB	ALA	B	278	23.881	29.171	-12.552	1.00	20.42
8541	C	ALA	B	278	25.990	28.377	-13.699	1.00	20.27
8542	O	ALA	B	278	26.607	27.383	-13.306	1.00	19.24
8543	N	ARG	B	279	25.819	28.639	-14.990	1.00	20.74
8545	CA	ARG	B	279	26.307	27.695	-15.997	1.00	21.12
8547	CB	ARG	B	279	25.765	28.003	-17.392	1.00	21.76
8550	CG	ARG	B	279	26.088	26.897	-18.402	1.00	22.89
8553	CD	ARG	B	279	25.654	27.222	-19.814	1.00	25.89
8556	NE	ARG	B	279	26.498	28.272	-20.382	1.00	26.63
8558	CZ	ARG	B	279	26.296	28.833	-21.562	1.00	26.13

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8559	NH1	ARG	B	279	25.253	28.490	-22.311	1.00	24.20
8562	NH2	ARG	B	279	27.138	29.760	-21.981	1.00	25.45
8565	C	ARG	B	279	27.831	27.650	-16.001	1.00	21.30
8566	O	ARG	B	279	28.416	26.590	-16.177	1.00	21.07
8567	N	ASP	B	280	28.461	28.795	-15.766	1.00	21.40
8569	CA	ASP	B	280	29.915	28.874	-15.595	1.00	21.87
8571	CB	ASP	B	280	30.335	30.327	-15.313	1.00	22.54
8574	CG	ASP	B	280	30.370	31.200	-16.579	1.00	25.24
8575	OD1	ASP	B	280	30.630	32.424	-16.457	1.00	28.05
8576	OD2	ASP	B	280	30.138	30.759	-17.724	1.00	26.91
8577	C	ASP	B	280	30.401	27.958	-14.456	1.00	21.04
8578	O	ASP	B	280	31.440	27.297	-14.562	1.00	20.76
8579	N	LEU	B	281	29.633	27.922	-13.372	1.00	20.21
8581	CA	LEU	B	281	29.994	27.151	-12.188	1.00	19.69
8583	CB	LEU	B	281	29.141	27.569	-10.992	1.00	19.82
8586	CG	LEU	B	281	29.530	28.953	-10.452	1.00	18.53
8588	CD1	LEU	B	281	28.423	29.532	-9.589	1.00	19.63
8592	CD2	LEU	B	281	30.812	28.869	-9.646	1.00	19.99
8596	C	LEU	B	281	29.838	25.670	-12.468	1.00	19.73
8597	O	LEU	B	281	30.671	24.889	-12.094	1.00	20.05
8598	N	ILE	B	282	28.774	25.295	-13.150	1.00	20.33
8600	CA	ILE	B	282	28.597	23.906	-13.555	1.00	21.14
8602	CB	ILE	B	282	27.190	23.672	-14.076	1.00	21.02
8604	CG1	ILE	B	282	26.178	23.925	-12.949	1.00	22.56
8607	CD1	ILE	B	282	26.532	23.265	-11.610	1.00	22.71
8611	CG2	ILE	B	282	27.041	22.244	-14.624	1.00	21.66
8615	C	ILE	B	282	29.659	23.477	-14.566	1.00	21.32
8616	O	ILE	B	282	30.149	22.359	-14.488	1.00	21.92
8617	N	ASP	B	283	30.032	24.358	-15.487	1.00	21.87
8619	CA	ASP	B	283	31.112	24.056	-16.430	1.00	22.32
8621	CB	ASP	B	283	31.436	25.261	-17.330	1.00	22.60
8624	CG	ASP	B	283	30.410	25.503	-18.417	1.00	23.70
8625	OD1	ASP	B	283	30.445	26.623	-18.989	1.00	26.27
8626	OD2	ASP	B	283	29.548	24.676	-18.786	1.00	22.23
8627	C	ASP	B	283	32.369	23.705	-15.624	1.00	22.25
8628	O	ASP	B	283	33.066	22.756	-15.928	1.00	21.47
8629	N	ASP	B	284	32.636	24.490	-14.588	1.00	22.34
8631	CA	ASP	B	284	33.793	24.291	-13.731	1.00	23.23
8633	CB	ASP	B	284	33.980	25.509	-12.820	1.00	23.34
8636	CG	ASP	B	284	35.161	25.368	-11.918	1.00	26.31
8637	OD1	ASP	B	284	36.305	25.530	-12.420	1.00	28.34
8638	OD2	ASP	B	284	35.037	25.088	-10.697	1.00	28.06
8639	C	ASP	B	284	33.670	22.986	-12.925	1.00	22.69
8640	O	ASP	B	284	34.641	22.234	-12.816	1.00	22.49
8641	N	ALA	B	285	32.474	22.703	-12.405	1.00	22.19
8643	CA	ALA	B	285	32.204	21.431	-11.725	1.00	22.57
8645	CB	ALA	B	285	30.752	21.361	-11.263	1.00	22.03
8649	C	ALA	B	285	32.524	20.233	-12.631	1.00	22.99
8650	O	ALA	B	285	33.151	19.270	-12.190	1.00	22.66
8651	N	ARG	B	286	32.115	20.321	-13.895	1.00	23.78
8653	CA	ARG	B	286	32.394	19.283	-14.883	1.00	25.16
8655	CB	ARG	B	286	31.628	19.550	-16.180	1.00	25.91

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8658	CG	ARG	B	286	30.138	19.170	-16.097	1.00	28.32
8661	CD	BARG	B	286	29.468	18.992	-17.466	0.35	29.52
8662	CD	AARG	B	286	29.453	19.007	-17.451	0.65	30.92
8667	NE	BARG	B	286	29.262	20.264	-18.163	0.35	29.83
8668	NE	AARG	B	286	28.271	18.146	-17.365	0.65	31.71
8671	CZ	BARG	B	286	28.839	20.386	-19.423	0.35	30.53
8672	CZ	AARG	B	286	28.231	16.856	-17.684	0.65	33.32
8673	NH1	BARG	B	286	28.567	19.313	-20.165	0.35	30.23
8674	NH1	AARG	B	286	29.309	16.209	-18.125	0.65	33.00
8679	NH2	BARG	B	286	28.688	21.596	-19.951	0.35	30.87
8680	NH2	AARG	B	286	27.089	16.195	-17.563	0.65	33.96
8685	C	ARG	B	286	33.894	19.108	-15.170	1.00	25.22
8686	O	ARG	B	286	34.349	17.988	-15.388	1.00	24.81
8687	N	GLN	B	287	34.651	20.204	-15.171	1.00	25.23
8689	CA	GLN	B	287	36.100	20.116	-15.322	1.00	25.93
8691	CB	GLN	B	287	36.756	21.497	-15.472	1.00	26.28
8694	CG	GLN	B	287	36.425	22.206	-16.775	1.00	29.31
8697	CD	GLN	B	287	37.009	21.533	-18.012	1.00	32.74
8698	OE1	GLN	B	287	38.047	20.880	-17.945	1.00	35.76
8699	NE2	GLN	B	287	36.340	21.706	-19.144	1.00	35.59
8702	C	GLN	B	287	36.706	19.364	-14.131	1.00	25.31
8703	O	GLN	B	287	37.565	18.521	-14.333	1.00	24.00
8704	N	SER	B	288	36.241	19.658	-12.905	1.00	25.12
8706	CA	SER	B	288	36.665	18.911	-11.720	1.00	25.39
8708	CB	SER	B	288	36.105	19.510	-10.414	1.00	25.38
8711	OG	SER	B	288	36.557	20.834	-10.215	1.00	24.82
8713	C	SER	B	288	36.289	17.433	-11.820	1.00	25.78
8714	O	SER	B	288	37.077	16.569	-11.459	1.00	25.49
8715	N	LEU	B	289	35.098	17.125	-12.321	1.00	26.38
8717	CA	LEU	B	289	34.709	15.726	-12.441	1.00	27.10
8719	CB	LEU	B	289	33.237	15.580	-12.838	1.00	26.93
8722	CG	LEU	B	289	32.258	15.977	-11.729	1.00	25.30
8724	CD1	LEU	B	289	30.821	15.804	-12.200	1.00	25.85
8728	CD2	LEU	B	289	32.524	15.189	-10.431	1.00	25.23
8732	C	LEU	B	289	35.635	14.995	-13.425	1.00	28.16
8733	O	LEU	B	289	35.998	13.854	-13.186	1.00	28.16
8734	N	LYS	B	290	36.053	15.677	-14.487	1.00	29.02
8736	CA	LYS	B	290	36.961	15.096	-15.481	1.00	30.79
8738	CB	LYS	B	290	37.313	16.118	-16.587	1.00	30.97
8741	CG	LYS	B	290	36.966	15.687	-18.011	1.00	33.97
8744	CD	LYS	B	290	36.614	16.900	-18.921	1.00	36.64
8747	CE	LYS	B	290	35.099	17.019	-19.182	1.00	37.79
8750	NZ	LYS	B	290	34.637	18.445	-19.343	1.00	38.84
8754	C	LYS	B	290	38.244	14.611	-14.809	1.00	31.28
8755	O	LYS	B	290	38.750	13.544	-15.141	1.00	31.44
8756	N	GLN	B	291	38.759	15.401	-13.869	1.00	32.13
8758	CA	GLN	B	291	39.978	15.054	-13.152	1.00	33.58
8760	CB	GLN	B	291	40.470	16.251	-12.326	1.00	33.80
8763	CG	GLN	B	291	40.818	17.493	-13.167	1.00	35.12
8766	CD	GLN	B	291	40.846	18.775	-12.353	1.00	36.83
8767	OE1	GLN	B	291	41.175	18.756	-11.168	1.00	36.95
8768	NE2	GLN	B	291	40.495	19.893	-12.985	1.00	38.40

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8771	C	GLN	B	291	39.800	13.810	-12.265	1.00	34.42
8772	O	GLN	B	291	40.764	13.098	-12.013	1.00	34.62
8773	N	LEU	B	292	38.577	13.568	-11.784	1.00	35.42
8775	CA	LEU	B	292	38.248	12.364	-10.999	1.00	36.35
8777	CB	LEU	B	292	36.931	12.542	-10.251	1.00	36.39
8780	CG	LEU	B	292	36.924	13.515	-9.082	1.00	36.49
8782	CD1	LEU	B	292	35.562	13.491	-8.411	1.00	36.85
8786	CD2	LEU	B	292	38.023	13.153	-8.101	1.00	36.84
8790	C	LEU	B	292	38.141	11.088	-11.820	1.00	37.54
8791	O	LEU	B	292	38.519	10.015	-11.352	1.00	37.33
8792	N	ALA	B	293	37.598	11.193	-13.028	1.00	38.95
8794	CA	ALA	B	293	37.635	10.088	-13.974	1.00	40.14
8796	CB	ALA	B	293	36.587	10.291	-15.078	1.00	40.36
8800	C	ALA	B	293	39.045	9.950	-14.565	1.00	40.76
8801	O	ALA	B	293	39.206	9.462	-15.677	1.00	41.94
8802	N	GLU	B	294	40.045	10.442	-13.834	1.00	41.22
8804	CA	GLU	B	294	41.456	10.118	-14.039	1.00	41.53
8806	CB	GLU	B	294	42.240	11.402	-14.318	1.00	41.94
8809	CG	GLU	B	294	43.620	11.186	-14.911	1.00	44.01
8812	CD	GLU	B	294	44.144	12.428	-15.604	1.00	45.96
8813	OE1	GLU	B	294	44.166	13.499	-14.953	1.00	48.06
8814	OE2	GLU	B	294	44.528	12.332	-16.794	1.00	47.73
8815	C	GLU	B	294	42.047	9.414	-12.808	1.00	40.89
8816	O	GLU	B	294	43.185	8.941	-12.846	1.00	41.57
8817	N	GLN	B	295	41.295	9.399	-11.705	1.00	39.90
8819	CA	GLN	B	295	41.549	8.516	-10.565	1.00	38.66
8821	CB	GLN	B	295	41.248	9.243	-9.243	1.00	38.65
8824	CG	GLN	B	295	41.958	10.592	-9.083	1.00	38.47
8827	CD	GLN	B	295	41.556	11.354	-7.816	1.00	37.66
8828	OE1	GLN	B	295	41.179	10.751	-6.807	1.00	36.11
8829	NE2	GLN	B	295	41.658	12.686	-7.867	1.00	36.75
8832	C	GLN	B	295	40.681	7.258	-10.689	1.00	37.75
8833	O	GLN	B	295	40.432	6.560	-9.698	1.00	37.50
8834	N	SER	B	296	40.220	6.995	-11.914	1.00	36.44
8836	CA	SER	B	296	39.373	5.852	-12.261	1.00	35.92
8838	CB	SER	B	296	40.117	4.541	-12.022	1.00	36.22
8841	OG	SER	B	296	39.666	3.572	-12.955	1.00	38.05
8843	C	SER	B	296	38.003	5.810	-11.566	1.00	34.56
8844	O	SER	B	296	37.551	4.753	-11.143	1.00	34.47
8845	N	LEU	B	297	37.330	6.952	-11.485	1.00	32.72
8847	CA	LEU	B	297	36.060	7.022	-10.773	1.00	31.10
8849	CB	LEU	B	297	36.114	8.107	-9.699	1.00	30.86
8852	CG	LEU	B	297	37.166	7.891	-8.611	1.00	30.39
8854	CD1	LEU	B	297	37.381	9.150	-7.786	1.00	30.04
8858	CD2	LEU	B	297	36.771	6.739	-7.721	1.00	30.69
8862	C	LEU	B	297	34.910	7.286	-11.724	1.00	30.21
8863	O	LEU	B	297	35.045	8.047	-12.684	1.00	29.81
8864	N	ASP	B	298	33.776	6.655	-11.425	1.00	28.91
8866	CA	ASP	B	298	32.541	6.834	-12.171	1.00	28.55
8868	CB	ASP	B	298	31.659	5.597	-12.005	1.00	28.67
8871	CG	ASP	B	298	30.377	5.661	-12.823	1.00	30.58
8872	OD1	ASP	B	298	30.141	6.682	-13.512	1.00	31.79

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8873	OD2	ASP	B	298	29.534	4.729	-12.815	1.00	33.35
8874	C	ASP	B	298	31.830	8.086	-11.662	1.00	27.64
8875	O	ASP	B	298	31.132	8.050	-10.649	1.00	26.94
8876	N	THR	B	299	32.007	9.187	-12.390	1.00	26.96
8878	CA	THR	B	299	31.424	10.478	-12.020	1.00	26.33
8880	CB	THR	B	299	32.352	11.615	-12.471	1.00	26.05
8882	OG1	THR	B	299	32.571	11.538	-13.882	1.00	27.18
8884	CG2	THR	B	299	33.740	11.457	-11.879	1.00	26.15
8888	C	THR	B	299	30.006	10.704	-12.588	1.00	25.98
8889	O	THR	B	299	29.464	11.785	-12.453	1.00	25.98
8890	N	SER	B	300	29.392	9.682	-13.176	1.00	25.39
8892	CA	SER	B	300	28.130	9.855	-13.906	1.00	25.11
8894	CB	SER	B	300	27.672	8.535	-14.531	1.00	25.29
8897	OG	SER	B	300	27.346	7.581	-13.529	1.00	27.52
8899	C	SER	B	300	27.004	10.479	-13.077	1.00	24.18
8900	O	SER	B	300	26.340	11.391	-13.553	1.00	23.89
8901	N	ALA	B	301	26.788	10.001	-11.850	1.00	23.33
8903	CA	ALA	B	301	25.756	10.590	-10.983	1.00	22.98
8905	CB	ALA	B	301	25.555	9.776	-9.736	1.00	22.98
8909	C	ALA	B	301	26.051	12.044	-10.605	1.00	22.43
8910	O	ALA	B	301	25.138	12.850	-10.585	1.00	21.51
8911	N	LEU	B	302	27.321	12.361	-10.309	1.00	22.10
8913	CA	LEU	B	302	27.705	13.698	-9.887	1.00	21.91
8915	CB	LEU	B	302	29.102	13.715	-9.268	1.00	21.74
8918	CG	LEU	B	302	29.295	12.964	-7.951	1.00	22.89
8920	CD1	LEU	B	302	30.736	13.126	-7.523	1.00	23.47
8924	CD2	LEU	B	302	28.338	13.420	-6.858	1.00	23.02
8928	C	LEU	B	302	27.651	14.663	-11.058	1.00	22.32
8929	O	LEU	B	302	27.411	15.858	-10.863	1.00	21.59
8930	N	GLU	B	303	27.861	14.144	-12.270	1.00	22.83
8932	CA	GLU	B	303	27.716	14.933	-13.480	1.00	23.58
8934	CB	GLU	B	303	28.227	14.192	-14.720	1.00	24.19
8937	CG	GLU	B	303	29.708	13.867	-14.789	1.00	27.75
8940	CD	GLU	B	303	30.025	12.941	-15.962	1.00	31.36
8941	OE1	GLU	B	303	29.515	13.205	-17.070	1.00	34.68
8942	OE2	GLU	B	303	30.758	11.938	-15.784	1.00	33.57
8943	C	GLU	B	303	26.241	15.247	-13.705	1.00	23.21
8944	O	GLU	B	303	25.897	16.382	-14.000	1.00	23.30
8945	N	ALA	B	304	25.378	14.238	-13.592	1.00	22.93
8947	CA	ALA	B	304	23.954	14.418	-13.865	1.00	23.17
8949	CB	ALA	B	304	23.219	13.063	-13.846	1.00	23.72
8953	C	ALA	B	304	23.348	15.383	-12.844	1.00	22.99
8954	O	ALA	B	304	22.530	16.240	-13.186	1.00	22.84
8955	N	LEU	B	305	23.786	15.250	-11.596	1.00	22.47
8957	CA	LEU	B	305	23.331	16.111	-10.518	1.00	22.39
8959	CB	LEU	B	305	23.841	15.623	-9.166	1.00	22.42
8962	CG	LEU	B	305	23.319	16.420	-7.973	1.00	23.49
8964	CD1	LEU	B	305	21.813	16.473	-7.938	1.00	26.09
8968	CD2	LEU	B	305	23.835	15.859	-6.701	1.00	25.91
8972	C	LEU	B	305	23.766	17.540	-10.732	1.00	21.68
8973	O	LEU	B	305	22.993	18.452	-10.511	1.00	21.68
8974	N	ALA	B	306	25.002	17.742	-11.173	1.00	21.62

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
8976	CA	ALA	B	306	25.507	19.094	-11.401	1.00	21.18
8978	CB	ALA	B	306	26.970	19.055	-11.829	1.00	20.99
8982	C	ALA	B	306	24.649	19.827	-12.437	1.00	21.29
8983	O	ALA	B	306	24.260	20.978	-12.221	1.00	20.84
8984	N	ASP	B	307	24.356	19.157	-13.557	1.00	21.52
8986	CA	ASP	B	307	23.462	19.700	-14.575	1.00	21.89
8988	CB	ASP	B	307	23.298	18.717	-15.749	1.00	22.19
8991	CG	ASP	B	307	24.484	18.721	-16.695	1.00	24.91
8992	OD1	ASP	B	307	25.217	19.734	-16.774	1.00	27.76
8993	OD2	ASP	B	307	24.754	17.744	-17.418	1.00	28.49
8994	C	ASP	B	307	22.091	19.989	-13.985	1.00	21.17
8995	O	ASP	B	307	21.517	21.065	-14.199	1.00	21.04
8996	N	TYR	B	308	21.566	19.037	-13.226	1.00	20.68
8998	CA	TYR	B	308	20.230	19.196	-12.667	1.00	21.00
9000	CB	TYR	B	308	19.804	17.946	-11.921	1.00	20.75
9003	CG	TYR	B	308	18.419	18.039	-11.344	1.00	21.19
9004	CD1	TYR	B	308	18.220	18.052	-9.966	1.00	20.91
9006	CE1	TYR	B	308	16.956	18.127	-9.432	1.00	21.89
9008	CZ	TYR	B	308	15.853	18.187	-10.268	1.00	24.30
9009	OH	TYR	B	308	14.587	18.254	-9.704	1.00	26.37
9011	CE2	TYR	B	308	16.020	18.192	-11.643	1.00	23.04
9013	CD2	TYR	B	308	17.299	18.112	-12.174	1.00	22.71
9015	C	TYR	B	308	20.145	20.397	-11.726	1.00	21.05
9016	O	TYR	B	308	19.109	21.018	-11.613	1.00	20.68
9017	N	ILE	B	309	21.239	20.713	-11.043	1.00	21.13
9019	CA	ILE	B	309	21.245	21.825	-10.102	1.00	21.51
9021	CB	ILE	B	309	22.635	21.881	-9.382	1.00	21.42
9023	CG1	ILE	B	309	22.663	20.817	-8.279	1.00	21.51
9026	CD1	ILE	B	309	24.007	20.664	-7.593	1.00	22.06
9030	CG2	ILE	B	309	22.891	23.256	-8.766	1.00	22.35
9034	C	ILE	B	309	20.874	23.159	-10.774	1.00	21.80
9035	O	ILE	B	309	20.237	24.017	-10.162	1.00	21.41
9036	N	ILE	B	310	21.245	23.328	-12.041	1.00	22.74
9038	CA	ILE	B	310	20.886	24.542	-12.765	1.00	23.55
9040	CB	ILE	B	310	22.148	25.209	-13.364	1.00	23.89
9042	CG1	ILE	B	310	22.714	24.400	-14.540	1.00	24.25
9045	CD1	ILE	B	310	23.776	25.141	-15.342	1.00	24.35
9049	CG2	ILE	B	310	23.190	25.406	-12.269	1.00	24.66
9053	C	ILE	B	310	19.799	24.344	-13.828	1.00	23.85
9054	O	ILE	B	310	19.400	25.315	-14.470	1.00	24.70
9055	N	GLN	B	311	19.319	23.110	-14.015	1.00	23.74
9057	CA	GLN	B	311	18.251	22.833	-14.990	1.00	23.91
9059	CB	GLN	B	311	18.584	21.602	-15.821	1.00	24.17
9062	CG	GLN	B	311	19.713	21.884	-16.815	1.00	26.77
9065	CD	GLN	B	311	20.172	20.670	-17.588	1.00	28.31
9066	OE1	GLN	B	311	21.115	20.760	-18.367	1.00	33.64
9067	NE2	GLN	B	311	19.520	19.540	-17.382	1.00	32.21
9070	C	GLN	B	311	16.887	22.687	-14.329	1.00	23.46
9071	O	GLN	B	311	15.857	22.873	-14.981	1.00	23.30
9072	N	ARG	B	312	16.889	22.369	-13.033	1.00	23.14
9074	CA	ARG	B	312	15.666	22.175	-12.249	1.00	22.83
9076	CB	ARG	B	312	16.010	21.784	-10.806	1.00	22.67

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9079	CG	ARG	B	312	16.722	22.887	-10.002	1.00	21.91
9082	CD	ARG	B	312	17.584	22.348	-8.871	1.00	20.80
9085	NE	ARG	B	312	18.319	23.405	-8.180	1.00	19.32
9087	CZ	ARG	B	312	17.807	24.145	-7.212	1.00	19.88
9088	NH1	ARG	B	312	18.559	25.083	-6.640	1.00	20.86
9091	NH2	ARG	B	312	16.547	23.956	-6.806	1.00	18.83
9094	C	ARG	B	312	14.826	23.434	-12.199	1.00	23.29
9095	O	ARG	B	312	15.361	24.542	-12.222	1.00	22.52
9096	N	ASN	B	313	13.513	23.232	-12.116	1.00	24.23
9098	CA	ASN	B	313	12.519	24.294	-11.967	1.00	25.30
9100	CB	ASN	B	313	11.404	24.132	-13.023	1.00	25.73
9103	CG	ASN	B	313	10.586	22.855	-12.843	1.00	27.06
9104	OD1	ASN	B	313	10.893	22.015	-12.003	1.00	30.28
9105	ND2	ASN	B	313	9.526	22.712	-13.642	1.00	30.33
9108	C	ASN	B	313	11.922	24.303	-10.550	1.00	26.15
9109	O	ASN	B	313	10.931	24.991	-10.282	1.00	26.07
9110	N	LYS	B	314	12.523	23.510	-9.663	1.00	26.76
9112	CA	LYS	B	314	12.057	23.349	-8.295	1.00	27.55
9114	CB	LYS	B	314	10.997	22.245	-8.214	1.00	28.24
9117	CG	LYS	B	314	11.437	20.876	-8.748	1.00	30.42
9120	CD	LYS	B	314	10.388	19.777	-8.483	1.00	34.02
9123	CE	LYS	B	314	9.281	19.733	-9.557	1.00	35.81
9126	NZ	LYS	B	314	9.763	19.297	-10.914	1.00	37.55
9130	C	LYS	B	314	13.212	23.017	-7.370	1.00	27.53
9131	O	LYS	B	314	13.045	23.018	-6.148	1.00	27.94
9132	OXT	LYS	B	314	14.311	22.729	-7.848	1.00	26.55
9133	O9	ipp	X	900	59.879	67.784	6.844	1.00	22.62
9134	P7	ipp	X	900	60.281	67.030	8.078	1.00	20.44
9135	O8	ipp	X	900	61.128	65.793	7.905	1.00	20.16
9136	O10	ipp	X	900	58.921	66.747	8.923	1.00	20.32
9137	P11	ipp	X	900	58.096	65.364	9.039	1.00	20.72
9138	O13	ipp	X	900	58.271	64.667	7.712	1.00	21.48
9139	O12	ipp	X	900	58.760	64.598	10.167	1.00	20.42
9140	O14	ipp	X	900	56.677	65.719	9.388	1.00	19.87
9141	O6	ipp	X	900	61.085	68.067	9.000	1.00	23.40
9142	C5	ipp	X	900	60.446	69.278	9.396	1.00	22.55
9145	C4	ipp	X	900	61.386	70.077	10.277	1.00	23.87
9148	C2	ipp	X	900	62.729	70.303	9.627	1.00	24.00
9149	C3	ipp	X	900	62.847	70.872	8.237	1.00	23.48
9153	C1	ipp	X	900	63.818	70.021	10.311	1.00	24.77
9156	O12	ris	X	901	57.820	74.304	11.572	1.00	21.28
9157	P9	ris	X	901	58.623	73.691	10.433	1.00	21.35
9158	O11	ris	X	901	58.329	74.511	8.992	1.00	22.29
9160	O10	ris	X	901	58.206	72.094	10.263	1.00	22.10
9162	C8	ris	X	901	60.334	73.798	10.791	1.00	20.58
9163	O13	ris	X	901	61.051	73.167	9.710	1.00	21.47
9165	P14	ris	X	901	60.832	75.467	10.955	1.00	21.49
9166	O16	ris	X	901	60.487	76.175	9.664	1.00	20.67
9167	O15	ris	X	901	60.014	76.127	12.259	1.00	20.29
9169	O17	ris	X	901	62.473	75.654	11.235	1.00	16.79
9171	C7	ris	X	901	60.517	73.036	12.110	1.00	20.01
9174	C2	ris	X	901	61.916	72.843	12.658	1.00	20.04

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9175	C1	ris X	901		62.030	72.693	14.038	1.00	22.23
9177	C6	ris X	901		63.284	72.496	14.614	1.00	21.92
9179	C5	ris X	901		64.396	72.454	13.790	1.00	21.90
9181	N4	ris X	901		64.272	72.597	12.461	1.00	20.50
9182	C3	ris X	901		63.073	72.787	11.887	1.00	20.38
9184	O9	ipp X	902		16.064	23.295	-2.975	1.00	21.48
9185	P7	ipp X	902		16.496	22.587	-1.731	1.00	20.32
9186	O8	ipp X	902		17.402	21.368	-1.817	1.00	20.60
9187	O10	ipp X	902		15.180	22.297	-0.852	1.00	19.29
9188	P11	ipp X	902		14.357	20.933	-0.731	1.00	21.41
9189	O13	ipp X	902		14.501	20.303	-2.099	1.00	21.14
9190	O12	ipp X	902		15.018	20.139	0.361	1.00	19.56
9191	O14	ipp X	902		12.943	21.318	-0.386	1.00	20.18
9192	O6	ipp X	902		17.282	23.658	-0.828	1.00	21.57
9193	C5	ipp X	902		16.665	24.901	-0.520	1.00	20.59
9196	C4	ipp X	902		17.539	25.684	0.451	1.00	20.72
9199	C2	ipp X	902		18.923	25.954	-0.086	1.00	20.12
9200	C3	ipp X	902		19.094	26.613	-1.425	1.00	20.10
9204	C1	ipp X	902		19.970	25.641	0.637	1.00	19.72
9207	O12	ris X	903		13.949	29.944	1.653	1.00	18.96
9208	P9	ris X	903		14.827	29.319	0.595	1.00	18.15
9209	O11	ris X	903		14.564	30.066	-0.891	1.00	17.76
9211	O10	ris X	903		14.479	27.699	0.371	1.00	17.12
9213	C8	ris X	903		16.543	29.484	1.000	1.00	16.83
9214	O13	ris X	903		17.268	28.905	-0.099	1.00	14.71
9216	P14	ris X	903		17.105	31.143	1.147	1.00	16.07
9217	O16	ris X	903		16.424	31.703	2.361	1.00	18.08
9218	O15	ris X	903		18.754	31.239	1.421	1.00	20.15
9220	O17	ris X	903		16.681	31.883	-0.303	1.00	17.24
9222	C7	ris X	903		16.736	28.711	2.310	1.00	15.64
9225	C2	ris X	903		18.144	28.461	2.843	1.00	17.89
9226	C1	ris X	903		18.231	28.146	4.193	1.00	17.51
9228	C6	ris X	903		19.477	27.908	4.776	1.00	17.87
9230	C5	ris X	903		20.612	27.985	3.980	1.00	18.68
9232	N4	ris X	903		20.535	28.281	2.665	1.00	18.45
9233	C3	ris X	903		19.332	28.506	2.084	1.00	18.77
9235	MG	MG X	904		15.574	31.310	-1.873	1.00	21.07
9236	MG	MG X	905		17.080	32.751	3.968	1.00	17.94
9237	MG	MG X	906		14.279	31.564	2.944	1.00	18.98
9238	MG	MG X	907		58.027	75.928	12.811	1.00	21.97
9239	MG	MG X	908		59.508	75.731	8.080	1.00	25.32
9240	MG	MG X	909		60.807	77.116	13.792	1.00	19.86
9241	OWO	HOH X	1		69.581	70.101	13.536	1.00	18.91
9244	OWO	HOH X	2		62.678	62.339	10.204	1.00	15.42
9247	OWO	HOH X	3		25.799	25.747	3.926	1.00	15.73
9250	OWO	HOH X	4		59.333	62.010	10.213	1.00	18.17
9253	OWO	HOH X	5		18.822	17.964	0.386	1.00	18.32
9256	OWO	HOH X	6		13.596	24.842	-2.548	1.00	13.98
9259	OWO	HOH X	7		60.443	70.120	5.487	1.00	20.05
9262	OWO	HOH X	8		67.024	68.022	10.947	1.00	18.31
9265	OWO	HOH X	9		75.891	66.532	13.529	1.00	16.24
9268	OWO	HOH X	10		61.389	59.407	28.540	1.00	15.76

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9271	OWO	HOH	X	11	16.713	25.479	-4.403	1.00	16.69
9274	OWO	HOH	X	12	17.228	19.008	-1.948	1.00	17.97
9277	OWO	HOH	X	13	60.948	63.338	7.816	1.00	17.21
9280	OWO	HOH	X	14	12.537	21.690	6.873	1.00	20.29
9283	OWO	HOH	X	15	17.395	34.432	2.680	1.00	15.95
9286	OWO	HOH	X	16	22.715	24.983	3.509	1.00	21.00
9289	OWO	HOH	X	17	23.103	23.679	1.175	1.00	16.66
9292	OWO	HOH	X	18	60.488	77.235	6.934	1.00	16.27
9295	OWO	HOH	X	19	57.327	69.233	7.233	1.00	17.06
9298	OWO	HOH	X	20	15.505	17.649	0.655	1.00	17.89
9301	OWO	HOH	X	21	34.673	22.728	-9.839	1.00	22.21
9304	OWO	HOH	X	22	12.191	23.940	-0.324	1.00	14.99
9307	OWO	HOH	X	23	4.461	26.280	19.031	1.00	23.20
9310	OWO	HOH	X	24	72.420	88.509	2.009	1.00	28.92
9313	OWO	HOH	X	25	73.365	71.690	24.882	1.00	15.83
9316	OWO	HOH	X	26	9.311	27.134	10.014	1.00	16.86
9319	OWO	HOH	X	27	33.303	4.388	14.111	1.00	23.61
9322	OWO	HOH	X	28	9.972	29.039	2.416	1.00	19.40
9325	OWO	HOH	X	29	20.315	24.167	4.178	1.00	21.86
9328	OWO	HOH	X	30	23.161	10.579	20.659	1.00	23.73
9331	OWO	HOH	X	31	62.889	76.521	13.608	1.00	18.10
9334	OWO	HOH	X	32	14.368	17.510	4.944	1.00	24.43
9337	OWO	HOH	X	33	31.222	26.334	11.934	1.00	21.87
9340	OWO	HOH	X	34	17.123	34.428	-0.050	1.00	18.82
9343	OWO	HOH	X	35	65.244	84.346	-6.827	1.00	23.12
9346	OWO	HOH	X	36	53.273	71.292	19.938	1.00	20.38
9349	OWO	HOH	X	37	75.108	70.654	21.698	1.00	19.01
9352	OWO	HOH	X	38	61.370	78.383	15.450	1.00	24.45
9355	OWO	HOH	X	39	64.170	68.585	13.753	1.00	23.11
9358	OWO	HOH	X	40	15.187	3.524	-3.226	1.00	21.48
9361	OWO	HOH	X	41	20.358	39.276	1.884	1.00	22.25
9364	OWO	HOH	X	42	59.729	80.370	3.839	1.00	25.41
9367	OWO	HOH	X	43	9.394	25.625	7.660	1.00	19.98
9370	OWO	HOH	X	44	19.279	13.591	19.445	1.00	25.74
9373	OWO	HOH	X	45	18.592	28.894	9.372	1.00	21.52
9376	OWO	HOH	X	46	16.733	32.742	-2.993	1.00	17.70
9379	OWO	HOH	X	47	28.337	35.553	9.793	1.00	24.55
9382	OWO	HOH	X	48	71.766	52.024	1.660	1.00	25.10
9385	OWO	HOH	X	49	5.509	18.812	21.857	1.00	25.11
9388	OWO	HOH	X	50	25.249	44.467	-11.635	1.00	22.90
9391	OWO	HOH	X	51	16.089	35.932	-5.867	1.00	20.15
9394	OWO	HOH	X	52	50.870	75.101	10.886	1.00	22.51
9397	OWO	HOH	X	53	58.111	59.051	3.773	1.00	23.52
9400	OWO	HOH	X	54	84.343	49.350	23.069	1.00	19.58
9403	OWO	HOH	X	55	56.087	75.553	13.615	1.00	15.17
9406	OWO	HOH	X	56	19.494	34.654	-1.382	1.00	20.86
9409	OWO	HOH	X	57	8.799	19.400	4.773	1.00	21.44
9412	OWO	HOH	X	58	39.726	12.512	12.694	1.00	37.61
9415	OWO	HOH	X	59	12.786	3.396	7.777	1.00	28.21
9418	OWO	HOH	X	61	33.547	28.085	-16.167	1.00	24.17
9421	OWO	HOH	X	62	60.548	68.421	32.431	1.00	22.66
9424	OWO	HOH	X	63	52.652	63.594	14.580	1.00	21.16

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9427	OWO	HOH	X	64	63.267	78.956	8.228	1.00	23.96
9430	OWO	HOH	X	65	21.674	40.154	-16.591	1.00	19.82
9433	OWO	HOH	X	66	62.524	73.265	19.235	1.00	24.72
9436	OWO	HOH	X	67	50.175	67.476	14.681	1.00	24.07
9439	OWO	HOH	X	68	16.317	24.542	22.592	1.00	24.88
9442	OWO	HOH	X	70	13.596	32.913	1.425	1.00	18.95
9445	OWO	HOH	X	71	33.743	4.683	-9.292	1.00	21.88
9448	OWO	HOH	X	72	84.877	52.105	15.691	1.00	35.89
9451	OWO	HOH	X	73	28.069	7.721	-7.921	1.00	22.28
9454	OWO	HOH	X	74	29.256	1.053	13.166	1.00	28.61
9457	OWO	HOH	X	75	26.790	-1.137	5.597	1.00	33.71
9460	OWO	HOH	X	76	33.840	27.398	-6.991	1.00	26.70
9463	OWO	HOH	X	77	20.039	38.545	-21.843	1.00	59.27
9466	OWO	HOH	X	78	49.910	55.142	25.447	1.00	26.46
9469	OWO	HOH	X	79	9.843	14.477	-1.615	1.00	27.96
9472	OWO	HOH	X	80	36.808	16.350	8.648	1.00	22.19
9475	OWO	HOH	X	81	43.245	14.999	0.753	1.00	22.13
9478	OWO	HOH	X	82	57.361	79.956	11.239	1.00	25.78
9481	OWO	HOH	X	83	9.775	24.342	-1.506	1.00	22.49
9484	OWO	HOH	X	84	68.131	69.501	22.346	1.00	28.17
9487	OWO	HOH	X	85	64.173	83.689	11.530	1.00	19.53
9490	OWO	HOH	X	86	58.920	48.042	6.438	1.00	22.32
9493	OWO	HOH	X	87	57.493	77.168	11.232	1.00	19.16
9496	OWO	HOH	X	88	77.326	71.627	2.643	1.00	27.72
9499	OWO	HOH	X	89	74.547	71.580	7.451	1.00	24.66
9502	OWO	HOH	X	91	48.469	59.380	21.046	1.00	23.24
9505	OWO	HOH	X	92	59.723	83.049	3.647	1.00	26.08
9508	OWO	HOH	X	93	29.853	24.288	-1.800	1.00	33.40
9511	O	HOH	X	94	56.128	56.547	-0.069	1.00	31.76
9514	O	HOH	X	95	60.992	57.155	5.055	1.00	25.17
9517	O	HOH	X	96	57.412	60.876	1.767	1.00	27.49
9520	O	HOH	X	98	10.425	34.341	14.720	1.00	25.28
9523	O	HOH	X	99	58.393	61.924	14.465	1.00	21.57
9526	O	HOH	X	100	15.514	40.203	-8.447	1.00	25.83
9529	O	HOH	X	101	71.395	44.872	6.706	1.00	23.21
9532	O	HOH	X	102	59.088	84.453	1.416	1.00	21.13
9535	O	HOH	X	103	10.805	35.476	2.484	1.00	30.21
9538	O	HOH	X	104	78.675	67.094	-0.168	1.00	30.94
9541	O	HOH	X	105	53.216	69.834	17.573	1.00	21.88
9544	O	HOH	X	106	11.540	21.193	-2.775	1.00	23.63
9547	O	HOH	X	107	56.434	66.036	16.603	1.00	21.18
9550	O	HOH	X	108	53.589	69.002	8.469	1.00	26.03
9553	O	HOH	X	109	22.171	2.588	12.364	1.00	25.07
9556	O	HOH	X	110	77.332	49.094	0.357	1.00	25.35
9559	O	HOH	X	111	33.771	36.319	-2.063	1.00	30.82
9562	O	HOH	X	112	12.214	37.251	-5.519	1.00	20.62
9565	O	HOH	X	113	68.012	47.978	18.112	1.00	22.53
9568	O	HOH	X	114	52.583	66.344	14.741	1.00	24.60
9571	O	HOH	X	115	54.317	78.524	24.510	1.00	28.76
9574	O	HOH	X	116	17.315	3.665	4.180	1.00	31.96
9577	O	HOH	X	117	41.900	14.903	-5.570	1.00	23.73
9580	O	HOH	X	118	25.232	6.606	-7.167	1.00	24.37

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9583	O	HOH	X	119	69.198	51.022	2.442	1.00	32.30
9586	O	HOH	X	120	54.454	75.970	7.898	1.00	29.61
9589	O	HOH	X	121	72.835	54.092	-0.028	1.00	28.37
9592	O	HOH	X	122	13.624	16.407	-7.904	1.00	26.27
9595	O	HOH	X	123	52.606	51.548	23.966	1.00	31.75
9598	O	HOH	X	124	64.545	60.261	-5.452	1.00	26.24
9601	O	HOH	X	125	48.485	73.411	29.403	1.00	35.53
9604	O	HOH	X	126	73.394	45.286	22.697	1.00	31.73
9607	O	HOH	X	127	1.619	16.387	23.748	1.00	35.87
9610	O	HOH	X	128	51.331	52.037	31.882	1.00	32.80
9613	O	HOH	X	130	59.702	84.785	5.880	1.00	28.09
9616	O	HOH	X	131	35.875	32.733	-2.230	1.00	41.90
9619	O	HOH	X	132	56.078	68.294	9.410	1.00	23.25
9622	O	HOH	X	133	68.940	88.925	-1.936	1.00	24.65
9625	O	HOH	X	134	66.234	47.041	21.983	1.00	27.75
9628	O	HOH	X	135	61.333	46.476	6.833	1.00	25.98
9631	O	HOH	X	136	67.556	54.792	30.084	1.00	27.45
9634	O	HOH	X	137	40.092	4.846	14.202	1.00	33.56
9637	O	HOH	X	138	6.434	23.324	4.635	1.00	23.23
9640	O	HOH	X	139	53.326	52.199	10.569	1.00	27.46
9643	O	HOH	X	140	16.797	40.699	-15.388	1.00	31.25
9646	O	HOH	X	141	55.505	68.569	5.472	1.00	31.05
9649	O	HOH	X	142	19.829	28.141	-14.550	1.00	32.03
9652	O	HOH	X	143	72.192	80.036	19.386	1.00	26.69
9655	O	HOH	X	144	49.567	62.818	10.675	1.00	36.36
9658	O	HOH	X	145	77.624	80.795	7.572	1.00	30.84
9661	O	HOH	X	146	70.251	84.697	14.333	1.00	29.10
9664	O	HOH	X	147	22.147	28.439	-15.860	1.00	25.06
9667	O	HOH	X	149	13.634	35.572	1.265	1.00	25.62
9670	O	HOH	X	150	82.244	46.629	23.769	1.00	35.68
9673	O	HOH	X	151	63.846	88.990	3.561	1.00	28.36
9676	O	HOH	X	152	64.405	73.293	-9.004	1.00	59.74
9679	O	HOH	X	153	19.585	44.233	-0.968	1.00	31.22
9682	O	HOH	X	154	17.128	12.637	-4.589	1.00	25.38
9685	O	HOH	X	155	5.113	33.908	7.713	1.00	38.08
9688	O	HOH	X	156	30.306	34.937	-7.899	1.00	34.44
9691	O	HOH	X	157	3.129	22.986	-4.541	1.00	39.21
9694	O	HOH	X	158	66.626	69.399	13.372	1.00	23.00
9697	O	HOH	X	159	63.446	57.641	29.205	1.00	27.23
9700	O	HOH	X	160	54.243	50.317	14.175	1.00	34.68
9703	O	HOH	X	161	66.368	78.182	-9.856	1.00	26.10
9706	O	HOH	X	162	53.159	57.048	10.179	1.00	27.95
9709	O	HOH	X	163	44.219	16.007	-6.192	1.00	25.11
9712	O	HOH	X	164	80.589	61.008	18.291	1.00	25.88
9715	O	HOH	X	165	28.989	38.706	2.563	1.00	25.75
9718	O	HOH	X	166	11.238	30.773	0.615	1.00	24.14
9721	O	HOH	X	167	53.608	73.127	12.234	1.00	26.24
9724	O	HOH	X	169	63.586	45.033	14.349	1.00	31.13
9727	O	HOH	X	170	77.596	48.785	23.097	1.00	26.73
9730	O	HOH	X	171	84.848	48.026	14.304	1.00	29.46
9733	O	HOH	X	172	4.265	15.315	11.290	1.00	29.33
9736	O	HOH	X	173	3.381	31.069	16.737	1.00	33.72

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9739	O	HOH	X	174	55.238	65.487	7.142	1.00	31.03
9742	O	HOH	X	175	9.341	26.913	-11.288	1.00	29.49
9745	O	HOH	X	176	53.199	53.483	20.584	1.00	32.49
9748	O	HOH	X	177	14.338	14.643	-5.988	1.00	23.99
9751	O	HOH	X	178	38.329	22.112	-11.565	1.00	45.14
9754	O	HOH	X	179	39.337	18.256	2.081	1.00	27.57
9757	O	HOH	X	180	56.191	81.845	4.467	1.00	30.98
9760	O	HOH	X	181	20.859	16.036	-15.248	1.00	24.19
9763	O	HOH	X	182	52.592	52.636	34.412	1.00	33.36
9766	O	HOH	X	183	8.751	22.025	4.991	1.00	21.08
9769	O	HOH	X	184	63.183	88.654	8.668	1.00	32.88
9772	O	HOH	X	185	23.296	39.123	11.088	1.00	28.53
9775	O	HOH	X	186	21.029	42.374	-4.623	1.00	40.24
9778	O	HOH	X	187	61.193	73.706	-5.808	1.00	35.26
9781	O	HOH	X	188	55.468	47.798	19.949	1.00	28.75
9784	O	HOH	X	189	35.734	28.370	-1.891	1.00	42.91
9787	O	HOH	X	190	28.941	9.752	-9.745	1.00	28.83
9790	O	HOH	X	191	60.836	85.243	-5.478	1.00	33.63
9793	O	HOH	X	193	85.606	61.921	11.265	1.00	33.58
9796	O	HOH	X	194	78.387	74.119	-1.722	1.00	50.78
9799	O	HOH	X	195	7.183	30.679	0.916	1.00	33.15
9802	O	HOH	X	196	32.652	28.076	-18.831	1.00	28.06
9805	O	HOH	X	197	53.948	51.530	21.729	1.00	30.16
9808	O	HOH	X	198	3.740	12.442	13.203	1.00	38.10
9811	O	HOH	X	199	81.671	47.299	9.794	1.00	39.29
9814	O	HOH	X	200	76.149	46.441	21.909	1.00	32.74
9817	O	HOH	X	201	61.151	42.663	13.748	1.00	62.81
9820	O	HOH	X	202	54.688	79.719	12.391	1.00	30.29
9823	O	HOH	X	203	51.275	79.190	10.957	1.00	40.83
9826	O	HOH	X	204	14.506	30.823	-3.503	1.00	21.42
9829	O	HOH	X	205	14.195	32.814	-1.332	1.00	19.33
9832	O	HOH	X	206	12.434	31.396	3.683	1.00	16.08
9835	O	HOH	X	207	18.969	32.213	3.765	1.00	20.53
9838	O	HOH	X	208	17.536	34.005	5.600	1.00	16.75
9841	O	HOH	X	209	33.461	39.878	0.879	1.00	48.09
9844	O	HOH	X	210	78.263	66.876	16.527	1.00	37.29
9847	O	HOH	X	211	80.975	67.293	15.894	1.00	39.50
9850	O	HOH	X	212	82.405	67.613	13.856	1.00	46.74
9853	O	HOH	X	213	50.671	57.527	11.069	1.00	40.42
9856	O	HOH	X	214	51.601	55.517	13.513	1.00	33.26
9859	O	HOH	X	215	62.729	54.517	30.771	1.00	40.62
9862	O	HOH	X	216	60.331	52.329	31.300	1.00	52.01
9865	O	HOH	X	217	31.078	32.997	-9.951	1.00	29.54
9868	O	HOH	X	218	33.614	33.829	-1.558	1.00	23.66
9871	O	HOH	X	219	3.882	31.855	12.746	1.00	38.99
9874	O	HOH	X	220	15.840	40.330	-3.855	1.00	26.18
9877	O	HOH	X	221	15.995	38.459	-6.211	1.00	24.53
9880	O	HOH	X	222	63.555	73.039	-4.552	1.00	36.76
9883	O	HOH	X	223	65.686	72.948	-6.046	1.00	30.87
9886	O	HOH	X	224	61.071	89.367	2.768	1.00	33.44
9889	O	HOH	X	225	85.368	50.306	25.290	1.00	39.68
9892	O	HOH	X	226	10.770	31.661	-1.862	1.00	30.59

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
9895	O	HOH	X	227	67.074	86.090	20.611	1.00	47.90
9898	O	HOH	X	228	72.225	82.393	20.309	1.00	28.15
9901	O	HOH	X	229	23.258	30.948	-19.639	1.00	37.49
9904	O	HOH	X	230	18.514	43.214	-15.138	1.00	25.15
9907	O	HOH	X	231	18.316	39.793	-17.580	1.00	30.27
9910	O	HOH	X	232	18.565	40.376	-20.157	1.00	27.88
9913	O	HOH	X	233	10.124	22.994	6.965	1.00	22.65
9916	O	HOH	X	234	40.682	5.559	16.461	1.00	35.43
9919	O	HOH	X	235	60.087	44.060	7.813	1.00	29.04
9922	O	HOH	X	236	65.753	46.800	19.256	1.00	33.55
9925	O	HOH	X	237	47.350	74.880	26.880	1.00	40.56
9928	O	HOH	X	238	48.590	70.295	28.815	1.00	22.47
9931	O	HOH	X	239	62.111	62.571	-5.691	1.00	41.29
9934	O	HOH	X	240	58.266	75.096	6.385	1.00	20.97
9937	O	HOH	X	241	57.930	77.196	8.555	1.00	21.06
9940	O	HOH	X	242	60.766	78.814	9.905	1.00	24.54
9943	O	HOH	X	243	61.087	78.751	12.516	1.00	17.96
9946	O	HOH	X	244	66.063	45.873	5.892	1.00	30.86
9949	O	HOH	X	245	68.834	44.595	6.140	1.00	27.12
9952	O	HOH	X	246	40.240	21.104	-0.696	1.00	29.77
9955	O	HOH	X	247	54.038	67.321	16.979	1.00	23.18
9958	O	HOH	X	248	6.161	36.828	-2.610	1.00	45.75
9961	O	HOH	X	249	32.414	42.931	-5.770	1.00	26.20
9964	O	HOH	X	250	8.263	18.675	-2.300	1.00	37.46
9967	O	HOH	X	251	57.682	88.576	6.524	1.00	41.67
9970	O	HOH	X	252	9.403	38.851	14.485	1.00	38.72
9973	O	HOH	X	253	7.150	40.262	16.390	1.00	45.72
9976	O	HOH	X	254	53.657	64.735	-1.870	1.00	50.87
9979	O	HOH	X	255	54.909	49.982	11.303	1.00	29.97
9982	O	HOH	X	256	54.469	48.142	15.766	1.00	35.94
9985	O	HOH	X	257	64.819	51.877	25.591	1.00	48.64
9988	O	HOH	X	258	48.466	60.211	34.761	1.00	34.69
9991	O	HOH	X	259	50.594	60.418	33.231	1.00	29.29
9994	O	HOH	X	260	44.303	61.380	23.666	1.00	50.60
9997	O	HOH	X	261	42.915	58.238	26.279	1.00	44.44
10000	O	HOH	X	262	52.554	63.196	6.954	1.00	45.59
10003	O	HOH	X	263	75.789	43.073	11.027	1.00	45.52
10006	O	HOH	X	264	63.099	46.831	5.108	1.00	38.28
10009	O	HOH	X	265	44.196	64.994	15.827	1.00	37.65
10012	O	HOH	X	266	43.951	62.363	16.102	1.00	46.48
10015	O	HOH	X	267	39.222	63.891	21.996	1.00	52.12
10018	O	HOH	X	268	42.850	63.664	23.396	1.00	50.80
10021	O	HOH	X	269	48.526	74.293	31.675	1.00	36.34
10024	O	HOH	X	270	67.670	48.672	31.258	1.00	51.39
10027	O	HOH	X	271	81.199	48.984	16.751	1.00	28.66
10030	O	HOH	X	272	79.911	47.943	14.775	1.00	31.46
10033	O	HOH	X	273	85.017	50.279	19.126	1.00	30.80
10036	O	HOH	X	274	64.657	81.303	10.384	1.00	30.96
10039	O	HOH	X	275	62.329	87.607	6.341	1.00	31.55
10042	O	HOH	X	276	64.640	86.808	5.080	1.00	34.11
10045	O	HOH	X	277	60.179	93.225	8.295	1.00	40.09
10048	O	HOH	X	278	73.593	79.168	1.381	1.00	35.41

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
10051	O	HOH	X	279	74.858	77.325	-0.481	1.00	41.75
10054	O	HOH	X	280	77.068	76.446	0.836	1.00	38.59
10057	O	HOH	X	281	74.159	76.085	-2.785	1.00	31.06
10060	O	HOH	X	282	79.283	78.702	16.390	1.00	38.20
10063	O	HOH	X	283	77.257	76.993	10.420	1.00	32.78
10066	O	HOH	X	284	77.239	78.246	8.067	1.00	37.50
10069	O	HOH	X	285	73.948	68.872	7.682	1.00	33.72
10072	O	HOH	X	286	77.608	62.256	8.543	1.00	45.53
10075	O	HOH	X	287	84.634	47.863	10.649	1.00	33.57
10078	O	HOH	X	288	89.171	59.221	10.145	1.00	51.60
10081	O	HOH	X	289	88.540	58.568	7.606	1.00	57.77
10084	O	HOH	X	290	44.965	73.834	1.582	1.00	48.13
10087	O	HOH	X	291	49.561	81.495	7.222	1.00	45.30
10090	O	HOH	X	292	70.469	68.660	-8.004	1.00	41.08
10093	O	HOH	X	293	81.881	67.174	-2.963	1.00	39.74
10096	O	HOH	X	294	77.288	57.817	-5.855	1.00	32.90
10099	O	HOH	X	295	76.204	60.286	-6.405	1.00	33.62
10102	O	HOH	X	296	72.178	51.978	-1.088	1.00	40.76
10105	O	HOH	X	297	69.367	55.952	-6.441	1.00	41.52
10108	O	HOH	X	298	66.145	60.092	-7.585	1.00	37.64
10111	O	HOH	X	299	58.836	67.727	-7.779	1.00	45.55
10114	O	HOH	X	300	13.363	3.105	-5.157	1.00	38.92
10117	O	HOH	X	301	13.794	2.664	-0.805	1.00	33.87
10120	O	HOH	X	302	15.442	1.396	0.758	1.00	53.73
10123	O	HOH	X	303	17.525	-0.047	0.589	1.00	35.96
10126	O	HOH	X	304	13.277	5.297	-9.056	1.00	41.07
10129	O	HOH	X	305	10.451	8.808	-4.245	1.00	33.55
10132	O	HOH	X	306	11.127	5.641	1.860	1.00	28.72
10135	O	HOH	X	307	17.465	2.139	-2.799	1.00	30.54
10138	O	HOH	X	308	19.535	2.393	-4.513	1.00	33.31
10141	O	HOH	X	309	9.312	12.628	0.396	1.00	37.60
10144	O	HOH	X	310	7.665	11.510	3.549	1.00	34.31
10147	O	HOH	X	311	6.051	11.080	6.071	1.00	39.84
10150	O	HOH	X	312	10.116	7.158	11.883	1.00	33.40
10153	O	HOH	X	313	9.385	9.324	10.796	1.00	36.05
10156	O	HOH	X	314	14.622	2.412	13.739	1.00	31.45
10159	O	HOH	X	315	13.037	2.160	16.038	1.00	41.01
10162	O	HOH	X	316	5.930	10.969	15.786	1.00	34.44
10165	O	HOH	X	317	4.581	9.801	22.907	1.00	46.13
10168	O	HOH	X	318	1.584	18.885	-1.559	1.00	52.72
10171	O	HOH	X	319	37.184	2.115	-2.954	1.00	43.48
10174	O	HOH	X	320	36.733	3.493	-6.561	1.00	45.09
10177	O	HOH	X	321	20.082	0.677	4.712	1.00	26.47
10180	O	HOH	X	322	20.457	8.134	16.042	1.00	46.78
10183	O	HOH	X	323	19.090	10.262	18.888	1.00	37.59
10186	O	HOH	X	324	24.214	25.499	12.581	1.00	29.01
10189	O	HOH	X	325	14.989	39.048	7.973	1.00	31.76
10192	O	HOH	X	326	11.756	39.045	9.415	1.00	50.88
10195	O	HOH	X	327	7.810	36.884	3.543	1.00	43.84
10198	O	HOH	X	328	3.242	25.497	-3.703	1.00	29.56
10201	O	HOH	X	329	1.219	33.875	16.266	1.00	46.56
10204	O	HOH	X	330	1.544	29.687	13.872	1.00	40.23

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
10207	O	HOH	X	331	-0.474	27.413	15.144	1.00	54.89
10210	O	HOH	X	332	4.337	28.953	19.199	1.00	36.94
10213	O	HOH	X	333	-1.539	27.356	11.980	1.00	45.30
10216	O	HOH	X	334	-2.107	24.658	12.397	1.00	38.86
10219	O	HOH	X	335	2.398	22.547	20.759	1.00	43.49
10222	O	HOH	X	336	4.084	16.237	25.067	1.00	35.34
10225	O	HOH	X	337	3.978	13.588	25.815	1.00	45.80
10228	O	HOH	X	338	3.094	17.271	27.390	1.00	40.72
10231	O	HOH	X	339	4.241	24.783	21.717	1.00	35.53
10234	O	HOH	X	340	37.329	4.276	7.908	1.00	35.31
10237	O	HOH	X	341	39.684	14.815	17.121	1.00	27.65
10240	O	HOH	X	342	36.317	20.283	10.218	1.00	40.32
10243	O	HOH	X	343	32.070	22.082	3.932	1.00	19.26
10246	O	HOH	X	344	32.703	24.069	5.500	1.00	30.65
10249	O	HOH	X	345	21.195	37.054	0.700	1.00	23.85
10252	O	HOH	X	346	26.360	48.147	-1.801	1.00	37.57
10255	O	HOH	X	347	23.190	43.465	-4.592	1.00	34.90
10258	O	HOH	X	348	18.440	43.181	-3.522	1.00	30.15
10261	O	HOH	X	349	15.607	42.903	-4.850	1.00	31.05
10264	O	HOH	X	350	13.692	44.194	-3.391	1.00	41.66
10267	O	HOH	X	351	31.128	44.045	-7.531	1.00	41.41
10270	O	HOH	X	352	31.689	47.433	-4.627	1.00	30.20
10273	O	HOH	X	353	32.993	49.163	-3.190	1.00	38.18
10276	O	HOH	X	354	27.426	44.095	-10.304	1.00	33.92
10279	O	HOH	X	355	43.796	13.725	3.108	1.00	23.99
10282	O	HOH	X	356	42.070	17.335	1.525	1.00	30.43
10285	O	HOH	X	357	43.287	19.448	0.553	1.00	33.75
10288	O	HOH	X	358	39.828	16.002	5.397	1.00	35.08
10291	O	HOH	X	359	38.165	17.818	4.577	1.00	37.82
10294	O	HOH	X	360	33.950	17.800	-1.148	1.00	45.50
10297	O	HOH	X	361	11.762	24.758	-4.528	1.00	31.90
10300	O	HOH	X	362	3.975	32.061	-8.760	1.00	36.38
10303	O	HOH	X	363	15.528	42.830	-7.772	1.00	35.25
10306	O	HOH	X	364	14.500	29.223	-15.075	1.00	41.38
10309	O	HOH	X	365	32.850	21.982	-18.707	1.00	37.44
10312	O	HOH	X	366	40.592	8.573	-5.209	1.00	37.21
10315	O	HOH	X	367	25.811	11.663	-16.176	1.00	30.06
10318	O	HOH	X	368	26.945	13.028	-17.719	1.00	49.20
10321	O	HOH	X	369	24.479	22.182	-17.748	1.00	49.87
10324	O	HOH	X	370	21.021	17.997	-19.491	1.00	46.80
10327	O	HOH	X	371	23.217	19.367	-20.360	1.00	51.32
10330	O	HOH	X	372	22.674	25.397	-19.288	1.00	43.41
10333	O	HOH	X	373	12.811	20.249	-12.633	1.00	35.30
10336	O	HOH	X	374	55.709	88.998	19.001	1.00	47.10
10339	O	HOH	X	375	54.100	84.683	17.666	1.00	43.29
10342	O	HOH	X	376	48.970	77.908	17.748	1.00	39.82
10345	O	HOH	X	377	41.899	65.707	18.118	1.00	46.67
10348	O	HOH	X	378	48.368	58.949	18.441	1.00	30.58
10351	O	HOH	X	379	48.070	56.991	22.120	1.00	35.54
10354	O	HOH	X	380	47.998	54.800	20.225	1.00	42.38
10357	O	HOH	X	381	50.349	57.710	17.797	1.00	39.16
10360	O	HOH	X	382	32.392	26.723	0.642	1.00	35.35

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
10363	O	HOH	X	383	30.720	27.097	-2.250	1.00	27.18
10366	O	HOH	X	384	37.015	26.821	2.778	1.00	49.37
10369	O	HOH	X	385	38.443	23.443	3.534	1.00	33.87
10372	O	HOH	X	386	38.669	19.697	6.394	1.00	36.31
10375	O	HOH	X	387	30.186	-3.337	5.179	1.00	43.04
10378	O	HOH	X	388	36.379	2.179	1.556	1.00	42.15
10381	O	HOH	X	389	41.111	3.324	0.448	1.00	36.90
10384	O	HOH	X	390	43.161	2.676	-1.085	1.00	38.66
10387	O	HOH	X	391	62.047	69.399	25.389	1.00	88.66
10390	O	HOH	X	392	64.141	69.344	27.823	1.00	41.19
10393	O	HOH	X	393	58.875	89.405	12.710	1.00	64.96
10396	O	HOH	X	394	52.351	74.162	-4.548	1.00	47.29
10399	O	HOH	X	395	53.730	70.282	-5.715	1.00	55.71
10402	O	HOH	X	396	47.666	76.863	1.325	1.00	34.63
10405	O	HOH	X	397	59.660	75.843	-9.785	1.00	41.09
10408	O	HOH	X	398	62.561	78.886	-9.940	1.00	50.51
10411	O	HOH	X	399	30.260	2.431	-11.763	1.00	34.80
10414	O	HOH	X	400	27.528	3.971	-14.875	1.00	45.91
10417	O	HOH	X	401	33.506	13.418	-15.971	1.00	38.77
10420	O	HOH	X	402	41.028	6.141	-7.128	1.00	49.46
10423	O	HOH	X	403	28.710	29.035	-18.837	1.00	26.44
10426	O	HOH	X	404	29.796	34.872	-15.688	1.00	37.98
10429	O	HOH	X	405	27.243	36.476	-15.645	1.00	37.96
10432	O	HOH	X	406	31.047	35.920	-10.224	1.00	55.58
10435	O	HOH	X	407	33.680	38.851	-7.405	1.00	50.01
10438	O	HOH	X	408	25.402	37.066	-19.531	1.00	37.00
10441	O	HOH	X	409	35.153	33.776	5.764	1.00	48.02
10444	O	HOH	X	410	35.151	34.064	2.494	1.00	34.05
10447	O	HOH	X	411	34.154	30.349	7.013	1.00	44.18
10450	O	HOH	X	412	8.762	37.486	1.397	1.00	38.43
10453	O	HOH	X	413	7.201	35.165	1.535	1.00	41.39
10456	O	HOH	X	414	26.384	40.391	4.437	1.00	36.18
10459	O	HOH	X	415	51.309	51.810	-0.301	1.00	39.62
10462	O	HOH	X	416	29.679	4.776	17.263	1.00	29.29
10465	O	HOH	X	417	28.029	5.806	20.001	1.00	42.73
10468	O	HOH	X	418	20.603	24.902	18.280	1.00	45.48
10471	O	HOH	X	419	56.231	57.185	2.974	1.00	32.25
10474	O	HOH	X	420	53.164	57.686	5.692	1.00	35.05
10477	O	HOH	X	421	65.428	51.862	28.325	1.00	40.33